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LETTER TO THE EDITOR

The exact location of partition function zeros, a new method for statistical mechanics

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Abstract. A new mathematical mechanism is proposed for locating exactly sections of the locus of the limiting distribution of partition function zeros for model systems in statistical mechanics. Illustrations and applications to the two-dimensional Ising model and the hard square lattice gas are given; the exact location of the branch point singularity for the hard square lattice gas on the negative activity z axis is conjectured to be the negative root of the polynomial

$$2z^6+9z^5+42z^4+90z^3+96z^2+27z+2$$

which is closest to the origin, $z=-0.119\,392\ldots$.

The purpose of this letter is to report on a new method for locating exactly portions of the curves formed by the limiting distribution of the zeros of partition functions in the lattice models of statistical mechanics. The general formulation of statistical thermodynamics in terms of the analytic structure of the grand canonical partition function Ξ was introduced by Yang (1952) and Yang and Lee (1952) in terms of the zeros of Ξ in the complex plane of the activity $z=e^{\beta\mu}$, where for a finite number of particles Ξ is a polynomial in z. This formulation carries over into many problems in statistical mechanics formulated as lattice models since the appropriate partition function on a finite lattice is also a polynomial in a suitably chosen variable, at least to within a simple analytic multiplying factor. Well known examples of this are all Ising type models and lattice gas models (Fisher 1965, Domb 1974, Wood 1975, Griffiths 1972). The new method proposed here is a mathematical mechanism for obtaining increasingly large portions of the limiting locus of the distribution of partition function zeros exactly, and is suggested by a study of the manner in which *both* the distribution and location of these zeros for the two-dimensional Ising model in the complex temperature plane are systematically constructed in terms of semi-infinite strips of the lattice. In a recent letter (Wood 1985), the author showed that the zeros of the general anisotropic Onsager solution could be constructed in terms of the eigenvalues of the transfer matrix (Onsager 1944). It is implicit in this work that exact portions of the locus (or of a continuous sheet distribution) can be obtained from the eigenvalues of *finite* transfer matrices for $n\times\infty$ strips of the quadratic lattice. The manner in which this construction occurs very strongly suggests a general mathematical mechanism for the process, and relates to the theory of algebraic functions.

As is well known, the partition function for a model system in the transfer matrix formalism is a simple symmetric function of its eigenvalues

$$Z=\lambda_1^n+\lambda_2^n+\ldots+\lambda_\Omega^n \tag{1}$$

where n is the number of periodic repeats (cyclically connected) of a portion of a lattice, thus for an $n \times m$ section (cyclically connected) of the quadratic lattice Ising model $\Omega = 2^m$. Z is of course an analytic function of real temperature and by a suitable choice of variable can be expressed as a polynomial. The eigenvalues however are algebraic functions and many of them possess branch point singularities in the complex temperature plane. These branch point singularities appear to be the mechanism by which the natural boundary of the limiting partition function per site is constructed through a sequence in which $\Omega \to \infty$. In the Onsager solution the pattern is very simple and also very beautiful. Here the eigenvalues of any $m \times \infty$ strip are in the form

$$\lambda_k = (2 \sinh 2K)^{m/2} \prod_{i=1}^{m} \exp(\pm\tfrac{1}{2}\gamma_{2i-1}), \qquad k = 1, 2, \ldots, 2^{m-1} \tag{2}$$

which is the set containing the maximum eigenvalue (K real), only an even number of negative signs are allowed, and

$$\cosh \gamma_r = s + s^{-1} - \cos(r\pi/m), \qquad s = \sinh 2K. \tag{3}$$

Thus the functions e^{γ_r} each have two branch points at $\cosh \gamma_r = \pm 1$ with a natural cut along the line segment

$$-1 \leqslant \cosh \gamma_r \leqslant 1 \tag{4}$$

in the $\cosh \gamma_r$ plane. This cut places s on a segment of the unit circle $s = e^{i\psi}$ defined by

$$-\sin^2(r\pi/2m) \leqslant \cos \psi \leqslant \cos^2(r\pi/2m). \tag{5}$$

Thus the limiting locus of zeros, which is the whole circle $s = e^{i\psi}$, is already discernable in the branch points (and their cuts) of the eigenvalues (2) of *finite* transfer matrices.

The $2 \times \infty$ strip for example has a 4×4 transfer matrix with a pair of eigenvalues which have branch points at

$$s = \exp(\pm i\pi/3) \qquad \text{and} \qquad s = \exp(\pm i2\pi/3) \tag{6}$$

with a cut along the unit circle over

$$\pi/3 < \psi < 2\pi/3 \qquad \text{and} \qquad -2\pi/3 < \psi < -\pi/3. \tag{7}$$

Now this pattern is clearly repeated for the sequence of $m \times \infty$ strips where the eigenvalues produce cuts

$$-1 \leqslant \cosh \gamma_r \leqslant 1, \qquad r = 1, 3, 5, \ldots, 2^{m-1} \tag{8}$$

which represent a sequence of overlapping arcs on the circle $s = e^{i\psi}$. In this way on the sequence $m = 1, 2, \ldots,$ *both* the exact location and a distribution of zeros is constructed, and in the limit $m \to \infty$ the circle segments will finally become the whole circle and intersect the real axis at the limiting branch points $s = \pm 1$ (ferro-, and antiferromagnetic critical points).

It is of course natural to expect such a simple and appealing picture to emerge in the Onsager solution since the model is after all exactly solved for any arbitrary $m \times n$ finite section of the lattice, however, a basic mathematical structure which underlies the above is suggested, which may have an origin in the theory of algebraic functions which connects the branch points of λ_k with the natural boundary of the maximum eigenvalue in the thermodynamic limit. The mathematical structure which summarises the above in its most concise form is that if $T_m(z)$ is the transfer matrix for some semi-infinite system of a size characterised by m with z some suitably chosen variable (not necessarily one in which Z is a polynomial), then the limiting distribution of zeros is in part traced out by the function

$$R_m(z, \phi) = 0, \qquad 0 \leq \phi \leq 2\pi \tag{9}$$

where $R_m(z, \phi)$ is the resolvent between the two polynomials in λ

$$|T_m(z) - \lambda I| = 0 \tag{10a}$$

and

$$|T_m(z)\, \mathrm{e}^{-\mathrm{i}\phi} - \lambda I| = 0. \tag{10b}$$

The branch points of the eigenvalues λ_k are at the limit $\phi \to 0$, and the function (9) traces out trajectories in the complex z plane emanating from the branch points and returning to them on completing the circle $\mathrm{e}^{\mathrm{i}\phi}$; thus in the Onsager case above, on the $2 \times \infty$ strip (9) traces out the two arcs

$$\sinh 2K = \mathrm{e}^{\mathrm{i}\psi}, \qquad |\cos \psi| < \tfrac{1}{2}.$$

Listed below are the results of applying this formalism to (a) the Ising model on the square net with screw boundary conditions, (b) the Ising model on the honeycomb and triangular lattices, (c) the hard square gas on the quadratic lattice; the details of the method and of these applications will be the subject of a further publication.

The above picture for the Ising model on the quadratic lattice when the toroidal boundary conditions are changed to screw boundary conditions (Krammers and Wannier 1941) is preserved; again a large portion of the locus appears at an early stage. With a screw pitch of 2 equation (9) in the $z = \mathrm{e}^{-2K}$ plane produces a large part of the two circles

$$z = \pm 1 + \sqrt{2}\, \mathrm{e}^{\mathrm{i}\psi} \tag{11}$$

(Fisher 1965). Branch points

$$z = 3/8 \pm \mathrm{i}\sqrt{7}/8 \qquad \text{and} \qquad z = -3/8 \pm \mathrm{i}\sqrt{7}/8 \tag{12}$$

are produced, and the cuts connecting each complex conjugate pair cover the circular arcs which avoid intersecting the real axis at the points $\sqrt{2} - 1$ and $-\sqrt{2} + 1$ but do intersect the real axis at the complex temperature points $z = \pm(1 + \sqrt{2})$. In this case one also observes that a hyperbolic extension of (9) to pure imaginary angles ϕ completes the two circles and adds the real line segments $|z| > 1$.

Syozi (1951) has given the eigenvalue structure of strip divisions of both the honeycomb and triangular lattices. The limiting distribution of zeros for these two lattices has so far only been inferred on the assumption that they are the singularities in the integrands of the integral expressions for the limiting partition function per site, namely

$$\frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} \ln[C - D(\cos \theta + \cos \phi + \cos(\theta + \phi))]\, \mathrm{d}\theta\, \mathrm{d}\phi \tag{13}$$

where, for the honeycomb lattice

$$C = 1 + \cosh^3 2K, \qquad D = \sinh^2 2K \tag{14}$$

and for triangular lattice

$$C = \cosh^3 2K + \sinh^3 2K, \qquad D = \sinh 2K. \tag{15}$$

On this assumption the locus of zeros for the honeycomb lattice in the $\cosh 2K$ plane has two sections, first a circle

$$\cosh 2K = 1 + e^{i\phi} \tag{16}$$

and secondly a line segment

$$-1 \leq \cosh 2K \leq \tfrac{1}{2}. \tag{17}$$

The locus for the triangular lattice is the same except it is in the $\coth 2K$ plane by duality. The solutions to (9) produce the same constructional picture as in the Onsager case, branch point pairs appear on the circle (16) with cuts connecting them along arcs which avoid the real axis, and also branch point pairs appear on the real $\cosh 2K$ axis, *but* now the cut produced by (9) traces out the *whole* of the line segment (17).

The hard square gas (quadratic lattice) model has been chosen as an example of a problem which, although simple in some sense, has so far resisted all efforts to obtain an exact solution (Baxter 1982, Baxter *et al* 1980, Wood and Goldfinch 1980, Gaunt and Fisher 1965). An application of (9) to this model suggests that the branch point singularity of $\Xi(z)$ in the thermodynamic limit lying on the negative real activity z axis has probably been located exactly by taking a $4\times\infty$ strip.

Firstly for a $2\times\infty$ lattice (9) produces two branch points at

$$z = -3-2\sqrt{2} \qquad \text{and} \qquad -3+2\sqrt{2} \tag{18}$$

with a cut which simply connects the two points along the negative axis. On moving up to a $4\times\infty$ system the first thing we notice is that this cut is again produced in the second largest block of $T_4(z)$ (using a cyclic group reduction to irreducible representations of T), and that the largest block which is of degree 3 produces branch points at the roots of the polynomial

$$z^8+4z^7+28z^6+64z^5+178z^4+212z^3+88z^2+16z+1 \tag{19}$$

which has two negative roots at

$$z=-1 \qquad \text{and} \qquad z=-0.125\,981\ldots \tag{20}$$

and three complex pairs at

$$-0.8806\pm3.4734\text{i}, \qquad -0.3328\pm3.0601\text{i}, \qquad -0.2236\pm0.1234\text{i}. \tag{21}$$

Here equation (9) is in general a polynomial of degree 12, and on rotating ϕ in (9) we may expect to trace out an exact portion of the limiting distribution; movement of the trajectory may well complete the whole negative axis cut. A natural limit point occurs where (9) becomes the polynomial

$$2z^6+9z^5+42z^4+90z^3+96z^2+27z+2, \tag{22}$$

which has two negative roots at

$$z=-0.119\,392\ldots \qquad \text{and} \qquad z=-0.250\,074\ldots. \tag{23}$$

The only estimate of the singularity in Ξ on the negative real axis is that of Gaunt and Fisher (1965) using low density expansions, which was

$$z=-0.1194\pm0.0002. \tag{24}$$

On this basis I suspect that this branch point is the exact root of (22) closest to the origin.

Since the generator (9) can be constructed by hand for low orders in a variety of models, for example the three-state scalar Potts model on the square lattice has a block in T_2 which is quadratic, it is possible to obtain polynomial generators of trajectories which are essentially the exact equations

$$z = z(\phi) \tag{25}$$

for sections of the limiting distribution. There is a real possibility of extending these in the form of a closed curve (using a hyperbolic form of (9))

$$y = y(x)$$

in the complex plane. In the Ising model case for example, it would be difficult to resist the thought that the distribution was in fact the whole circle in the s plane! From a computational viewpoint much greater possibilities present themselves since the orbits under (9) can be computed for quite large transfer matrices, using group operations which leave the Hamiltonian invariant; an application to the three-dimensional Ising model is well within range. A full account of the work in this letter will appear elsewhere and application of the method to a variety of model systems is presently in progress.

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