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Algebraic approximations to the locus of partition function zeros

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Abstract. Applications of the mathematical formalism put forward in the previous paper are made to a number of well known lattice models in statistical mechanics. Sequences of algebraic curves are obtained from the branches of an algebraic function Λ_1, where Λ_1^+ at real temperatures is the branch of Λ_1 which is the partition function per site of an $m \times \infty$ lattice section. These sequences are viewed as approximations to parts of the limiting locus C_∞ of partition function zeros. Approximations to critical points can be obtained in a natural extension of these curves beyond the branch points of Λ_1^+.

1. Introduction

In the previous paper Wood (1987, hereafter referred to as I) has put forward a mathematical formalism which attempts to describe the way in which the limiting locus of partition function zeros C_∞ for the one-parameter lattice models of statistical mechanics is approached via an infinite sequence of algebraic curves C_m^{1+} generated by the connection curves of the eigenvalues of the block matrix τ_1, for $m \times \infty$ lattice sections. The partition function per site Λ_1^+ at real temperatures is a branch of the algebraic function Λ_1 defined by the characteristic equation of τ_1 and C_m^{1+} denotes the locus of points where the eigenvalues of τ_1 are simultaneously maximum and equal in modulus. It is envisaged that Λ_1^+ on a sequence of m has increasingly many branch points in the complex temperature plane which yield a system of near overlapping connection curves convergent upon C_∞. In the present paper we define a very natural extension of the connection curves C_m^{1+} beyond the branch points. Such extensions generate intersections with the real positive temperature axis which form a convergent sequence of approximations to the critical point. In the few cases of two-dimensional models where the eigenvalues of τ_1 or of the whole transfer matrix T_Ω have simple invariance symmetries under an analytic transformation of the temperature variable (or other variables), at arbitrary values of m Λ_1^+ can have branch points on an invariant curve which also corresponds to our proposed extension of C_m^{1+} through the complex branch points, and which is obtained at any specific value of m; the critical point is then obtained exactly. The duality and spin-field reversal symmetries of the general spin Ising models are both examples of this.

Since for the most part C_∞ is unknown, the validity of the formalism outlined in I in the present work can only be inferred from the accuracy of the approximations to the critical point obtained from the above extensions of C_m^{1+}. In addition to this, in the present examples where calculations have been performed for a few consecutive m values, the sequences of 'near' overlapping arc sections referred to above would appear to be a reasonable description of the outcome. All the calculations reported here have been performed exactly in the sense that the resolvents which define C_m^{1+} have been obtained exactly. An extension of the present calculations to larger values of m can be developed in a purely numerical way and these calculations will be reported elsewhere. In § 2 we describe the algebraic computation of C_m^{1+} and its extension beyond the branch points. The subsequent sections are specific applications to the following models: the q-state Potts model on the square and triangular lattices (§ 3), a non-planar two-dimensional Ising model (§ 4), the spin-1 Ising model on the square lattice (§ 5), the three-dimensional Ising model (§ 6), models with three-spin interactions present (§ 7), the general spin Ising model in a magnetic field (§ 8) and the hard square and hard hexagon gases and the chromatic polynomial of the plane triangular lattice (§ 9).

2. Algebraic approximations to C_∞ and critical points

The hypothesis represented by the equation

$$C_\infty = \lim_{m\to\infty} C_m^{1+} \tag{1}$$

(see (54) in I) can be used to form sequences of algebraic curves forming approximations to both the limiting locus of partition function zeros C_∞ and critical points. Given any one-parameter model, for a finite value of m we can obtain the branch points and the connection curves C_m^1 of the algebraic function $\Lambda_1(z)$ from the resolvent $R(z, h)$ defined in I where $|h| = 1$. We are interested in those connection curves C_m^{1+} which originate from the branch points of Λ_1^+ and form a set of connections between these branch points. At the outset we do not know which subset of C_m^1 belongs to C_m^{1+}. An examination of the eigenvalues of $\tau_1(z)$ at each branch point and at intersection points is usually sufficient to identify C_m^{1+}.

Following I (see § 4 of I) values of z on the curves belonging to C_m^{1+} and connecting branch points can be identified with the existence of a real quadratic factor of the characteristic equation of $\tau_1(z)$:

$$y^2 + b(z)y + c(z) = 0 \tag{2}$$

where Λ_1^+ is a multiple of one of the roots of (2) given by $\Lambda_1^+ = uy$, where $|u| = 1$. In (2) the values of z are those of one of the algebraic functions $z_i(h)$ generated by the resolvent, and the coefficients b and c are real in the domain $|h| = 1$. Those branch points of Λ_1^+ connected by $z_i(h)$ are the points $z_i(1)$ where (2) reduces to a perfect square. The connection curves and the resolvent are naturally mapped out in terms of the real variable

$$w = \tfrac{1}{2}(h + h^{-1}) = \cos\phi \tag{3}$$

where the domain $|h| = 1$ is the domain $-\pi \leq \phi \leq \pi$. In terms of w the quadratic factors (2) can be analytically extended to include the whole positive real line of w. This extended range corresponds to the range

$$|h| = 1 \qquad h \text{ real} \tag{4}$$

or equivalently adding the extension $\phi \to \mathrm{i}\phi$ to (3). Extending the connection curves into the extended domain of h in (4) is a very natural analytic extension since the quadratic factors (2) remain real quadratic factors over the whole of the extended domain. In the extended domain the connection curves C_m^{1+} are continued smoothly through the branch points and some of the extended curves intersect the real positive z axis at a specific value h_c. Beyond h_c the extended connection curves simply mark out a trajectory along the real axis. The intersection point on the real z axis from at least one extended curve forms an approximation to the critical point. For $|h|=1$, $z_i(h)$ consists of a complex conjugate pair of algebraic curves; in the extended domain the complex conjugate pair move on a curve which meets at the real axis point $z_i(h_c)$ and hence this point is a multiple root (of at least multiplicity 2) of the resolvent $R(z, h)$ and h_c is a branch point of the branch $z_i(h)$. Thus the approximations $z_i(h_c)$ to the critical point can be found precisely from the discriminant of the polynomial $R(z, h)$ which will locate the branch points of the algebraic function $Z(h)$ in the h plane. One or more such branch points will be on the real positive h axis and correspond to the intersections of the extended curves C_m^{1+} with the real positive z axis at $z_i(h_c)$. These intersection points can be computed exactly from the roots of the resolvent. At $h=h_c$ the branch $z_i(h)$ is non-analytic and an alternative determination of $z_i(h_c)$ is possible by finding the roots of the equation

$$\mathrm{d}h/\mathrm{d}z=0 \qquad \text{or} \qquad \mathrm{d}w/\mathrm{d}z=0. \tag{5}$$

The scheme above can be illustrated by an application to the nearest-neighbour two-dimensional Ising model on the simple quadratic lattice and the triangular lattice where C_∞ is known exactly. The advantages of using the Ising model for illustrative purposes are that Onsager's solution allows us to take m arbitrary and provides a basis of what to expect in dealing with other models. For the simple quadratic lattice Λ_1^+ for an arbitrary value of m is given by

$$\Lambda_1^+=(2s)^{m/2}\prod_{k=1}^{m}\exp(\gamma_{2k-1}/2) \qquad (s=\sinh 2K) \tag{6}$$

where

$$\cosh\gamma_r=s+s^{-1}-\cos r\pi/m \qquad (\gamma_r=\gamma_{2m-r}) \tag{6a}$$

and Λ_1^+ is a branch of Λ_1 generated by the characteristic equation τ_1. A branch point set of Λ_1^+ is readily identified; taking positive signs for all the γ in (6) except for γ_r and γ_{2m-r} which are chosen to have negative signs, we define an eigenvalue Λ_r. Clearly

$$\Lambda_1^+/\Lambda_r=\mathrm{e}^{2\gamma_r} \tag{7}$$

and hence $\gamma_r=0$ and $\gamma_r=\mathrm{i}\pi$ locate branch points of Λ_1^+ at a value of s given by the roots of the equation

$$\pm 1=s+s^{-1}-\cos r\pi/m \tag{8}$$

which are the complex conjugate pairs

$$s=\cos^2\frac{r\pi}{2m}\pm\mathrm{i}\left(1-\cos^4\frac{r\pi}{2m}\right)^{1/2} \tag{9a}$$

and

$$s=-\sin^2\frac{r\pi}{2m}\pm\mathrm{i}\left(1-\sin^4\frac{r\pi}{2m}\right)^{1/2} \tag{9b}$$

on the unit circle $s = e^{i\psi}$. Thus as m increases Λ_1^+ has an increasing number of branch points all lying on the unit circle $|s| = 1$. The connection curves over the branch points in (9) are simply obtained by setting $\gamma_r = i\phi$ in (7) which corresponds to the domain $|h| = 1$ in (4) and are the curves obtained by the algebraic functions $s(y)$ defined by the equation

$$y = s + s^{-1} - \cos r\pi/m \qquad -1 \leqslant y \leqslant 1 \tag{10}$$

which are the two complex conjugate arcs of the circle $|s| = 1$ joining the two branch points in (9) lying in the upper half plane and the two in the lower half plane. As m increases the connection curves C_m^{1+} of τ_1 form a system of overlapping arcs on $|s| = 1$, none of which intersect the real axis. The algebraic functions $s(y)$ are branches of a resolvent $R(s, h)$ and, using (10), we can observe the extension of the connection curves in the extended domain of (4), where (10) becomes

$$y = s + s^{-1} - \cos r\pi/m \qquad y \text{ real} \tag{11}$$

and the algebraic curves $s(y)$ now cover the whole of the circle $|s| = 1$. The critical point s_c is the intersection of $s(y)$ with the real axis, occurring at a branch point of $s(y)$ which has two branch points at

$$y = -\cos(r\pi/m) \pm 2 \tag{12}$$

corresponding to the points $s = \pm 1$. Alternatively (5) yields

$$s^2 = 1. \tag{13}$$

In this example the branch points of Λ_1^+ obtained for any finite value of m already lie on the limiting locus of partition function zeros where for all m the unit circle $|s| = 1$ is an invariant in the domain (4) of the algebraic curves $s(y)$. This invariance is a feature promoted by the self-duality of the model, which in this formalism is seen as a symmetry restricting the connection curves C_m^{1+} to lie on the same curve for all values of m. This mechanism is fully discussed in the following section in relation to the behaviour of the general q-state Potts model. In terms of approaching the problem with a finite transfer matrix, consider again the simple quadratic Ising model but now with screw boundary conditions imposed (Domb 1949a, b). With a screw pitch of two the transfer matrix is given by

$$T_4(z) = \begin{pmatrix} 1 & 0 & z & 0 \\ z^2 & 0 & z & 0 \\ 0 & z & 0 & z^2 \\ 0 & z & 0 & 1 \end{pmatrix} \qquad z = e^{2K}. \tag{14}$$

In general there is no cyclic symmetry present with screw boundary conditions and consequently, instead of obtaining a block τ_1, we deal with the whole transfer matrix and consider the connection curves of the resolvent $R_4(z)$. The characteristic equation of T_4 is in fact reducible into the two quadratic factors:

$$\Lambda^2 - \Lambda(1 + z) - z(z^2 - 1) = 0 \tag{15a}$$

$$\Lambda^2 - \Lambda(1 - z) + z(z^2 - 1) = 0. \tag{15b}$$

The branch points of the eigenvalues in (15a) and (15b) are at $z = \frac{3}{8} \pm i\sqrt{7}/8$ and $z = -\frac{3}{8} \pm i\sqrt{7}/8$, respectively, which are points on the two circles $z = -1 + \sqrt{2}\, e^{i\theta}$ and $z = 1 + \sqrt{2}\, e^{i\theta}$, respectively. It is easily verified that the branches $z(h)$ obtained from resolvents $R(z, h)$ constructed for each of (15a) and (15b) in the domain (4) trace out in full each of these two circles which are the limiting locus in the z plane (Fisher 1965). Again self-duality symmetry for an arbitrary screw pitch m determines that the two circles are invariants in the connection curves for each value of m.

For a further illustration consider the Ising model on the triangular lattice, where for $m = 2$ the characteristic equation of τ_1 is given by

$$\Lambda_1^2 - z^2(z^4+3)\Lambda_1 + z^2(z-1)^2 = 0 \qquad (z = \mathrm{e}^{2K}) \tag{16}$$

one root of which is Λ_1^+. For a quadratic equation with two roots λ_1 and λ_2 the branches $z_i(h)$ obtained from the resolvent in the domain (4) are the roots of the equation

$$2y = \frac{\lambda_1 + \lambda_2}{(\lambda_1\lambda_2)^{1/2}} \qquad (y \text{ real}) \tag{17}$$

where the domain $|y| \leq 1$ corresponds to $|h| = 1$ in (4). The branch points are the roots of (17) at $y = \pm 1$. The branch points of Λ_1 in (16) are the complex conjugate pair

$$z^2 = 1 \pm 2\mathrm{i} \tag{18}$$

and an isolated branch point at $z^2 = -1$. In the z^2 plane the extended connection curve is given by

$$z^2 = y \pm (y^2 - 2y - 3)^{1/2} \tag{19}$$

which for $-1 \leq y \leq 3$ is the circle

$$z^2 = 1 + 2\,\mathrm{e}^{\mathrm{i}\theta}. \tag{20}$$

The connection curve itself is the arc of (20) connecting the points in (18) and passing through $z^2 = -1$. The limiting locus of partition function zeros for the triangular lattice is the circle (20) and the real line segment $-1 \leq z \leq 0$ (van Saarloos and Kurtze 1984, Wood 1985). Thus we see that in the new formalism the circle (20) has again been obtained exactly from the finite case of $m = 2$, where the exact critical point of the model at $z_c^2 = 3$ is obtained from the 2×2 block $\tau_1(z)$. However in this case the model is not self-dual and reference to the q-state Potts model in § 3 shows that on the triangular lattice the case $q = 2$ is the only case where the critical point z_c is obtained exactly in the extended domain (4).

Although these examples illustrate the algebraic basis of the computations they are not typical of the hypothesis represented by (1) in that the domain of (4) has obtained the limiting locus exactly for m finite. Our expectation in general is that in the absence of symmetry which is independent of m the extended connection curves on a sequence of increasing m will converge onto C_∞. In this process branch points of Λ_1^+ will produce the connection curves C_m^{1+} which will form approximately overlapping arc lengths in the convergence to C_∞, and the extensions of these connection curves in the domain (4) will produce approximations to the critical point z_c. These two features (particularly the latter) are our guide in an initial assessment of the scheme when applied to models where C_∞ is not known, which of course is practically all cases. The appearance of extended connection curves which are invariants on a sequence of increasing m, as in the Ising model above, are possible when either the matrix $\tau_1(z)$ or the whole transfer matrix possesses a simple algebraic symmetry which is transformed into analytic symmetries in the polynomial coefficients $\phi_j(z)$ of λ^{n-j} in the characteristic equation. Self-duality is an example of such a symmetry but similar effects are observed from different symmetries; examples are found in the general spin Ising model in a magnetic field and in the monomer-dimer problem.

3. The two-dimensional q-state Potts model

The q-state Potts model on the simple quadratic lattice possesses self-dual symmetry where for a lattice of mn sites with toroidal boundary conditions the partition function $Z_{mn}(q, K)$ satisfies the simple relation

$$Z_{mn}(q, K) = \left(\frac{(e^K - 1)}{\sqrt{q}}\right)^{2mn} Z_{mn}(q, K^*) \tag{21}$$

where K and K^* are related by

$$(e^K - 1)(e^{K^*} - 1) = q \tag{22}$$

(for a review of duality relations and the Potts models see Wu (1982)). Writing (21) in the form

$$Z_{mn}(q, u) = u^{2mn} Z_{mn}(q, u^{-1}) \tag{23}$$

where $u = (e^K - 1)/\sqrt{q}$ we observe that $\Lambda_1^+(z)$ $(z = e^K)$ when mapped out in terms of the variable u satisfies the relation

$$\Lambda_1^+(q, u) = u^{2m} \Lambda_1^+(q, u^{-1}). \tag{24}$$

Now Λ_1^+ is a branch of the algebraic function Λ_1 defined by the characteristic equation of $\tau_1(z)$ and (24) applies to each branch of Λ_1. It follows from this that for any value of m where the irreducible characteristic equation of τ_1 is represented by

$$\sum_{r=0}^{s} \phi_r(u) \Lambda_1^{s-r} \qquad (\phi_0 = 1) \tag{25}$$

the coefficients ϕ_r which are polynomials in u satisfy the relation

$$\phi_r(u) = u^r \Phi_r(u) \tag{26}$$

where

$$\Phi_r(u) = \Phi_r(u^{-1}) \tag{27}$$

and hence the polynomials Φ_r can be transformed into polynomials in the variable $u + u^{-1}$. We see immediately that the circles $|u| = 1$, and u real for all q and all m, will be generated by the extended connection curves in the domain (4) formed from the resolvent $R(z, h)$ constructed from (25). This follows trivially since on $|u| = 1$ and u real the branches of $\Lambda_1(z)$ are either real or occur in constant multiples of complex conjugate pairs. The branch points of Λ_1^+ cannot lie on the positive real axis and hence are clearly likely to lie on the circle $|u| = 1$; we have recovered precisely the same invariance phenomena described for the $q = 2$ case above. Again branch points will occur on the unit circle $|u| = 1$ and for increasing m connection curves will form systems of arcs. For each m the domain (4) produces the whole circle. Given that Λ_1^+ has branch points on $|u| = 1$ then the arcs connecting these points are part of C_m^{1+}, namely the limiting locus of zeros of the block partition function of the $m \times \infty$ strip. In the limit of $m \to \infty$ at least one of these branch point pairs converge to the critical point $z_c = 1 + \sqrt{q}$. The argument above only identifies the arcs on $|u| = 1$ as part of C_m^{1+}; clearly the whole of C_m^{1+} can involve other curves not revealed by the duality symmetry. An interesting observation on the mathematical consequences of the duality symmetry is that on $|u| = 1$ branches of Λ_1 other than Λ_1^+ will trace out the circles $|u| = 1$ on the domain (4). That is to say that a complex conjugate pair of eigenvalues (to within a constant multiple) obtained from (25) and which are not on C_m^{1+} are also related to a branch point system with the connection curves of (4) tracing out all of $|u|=1$. This example therefore suggests that at branch points where the two eigenvalues are equal but *not* of maximum modulus the connection curves on (4) may prove worth considering, particularly if the extended curves have an intersection point with the real axis close to the critical point (see the spin-1 Ising model in § 5).

The algebraic effects described above are all illustrated by taking the smallest value of $m=2$. Here the characteristic equation of $\tau_1(z)$ is given in equation (9) of I which in terms of the variable u is given by

$$\Lambda_1^2-u^2[q^2(u^2+u^{-2})+q(6+q)+4q\sqrt{q}(u+u^{-1})]\Lambda_1+u^4[q(1+q)+q\sqrt{q}(u+u^{-1})]^2=0. \tag{28}$$

Hence Λ_1 is of the form $\Lambda_1=u^2\lambda$ where on $|u|=1$ and the real axis the roots $\lambda(u)$ are either real or complex conjugate pairs. Writing $w=(u+u^{-1})$, the branch points of Λ_1^+ occur at roots of the equation

$$q^2(w^2-2)+q(6+q)+4q\sqrt{q}w=y[2q(1+q)+2q\sqrt{q}w] \tag{29}$$

at $y=\pm 1$. On taking $y=1$ in (29) branch points occur on the unit circle $u=e^{i\theta}$ at values of θ given by

$$2\cos\theta=-\frac{1}{\sqrt{q}}\pm\sqrt{3}\left(1-\frac{1}{q}\right)^{1/2} \tag{30}$$

representing two complex conjugate pairs. The branch points at $y=-1$ are not on $|u|=1$; they are given by

$$w=-\frac{3}{\sqrt{q}}\pm i\sqrt{3}\left(1-\frac{1}{q}\right)^{1/2} \tag{31}$$

and yield an additional pair of connection curves belonging to C_2^{1+}. It is to be expected that curves other than $|u|=1$ belonging to C_m^{1+} will show an odd-even effect on m. The significance of these contributions to C_m^{1+} requires further numerical investigation. The full set of connection curves for $m=2$ and $q=3$ is shown in figure 1, where the

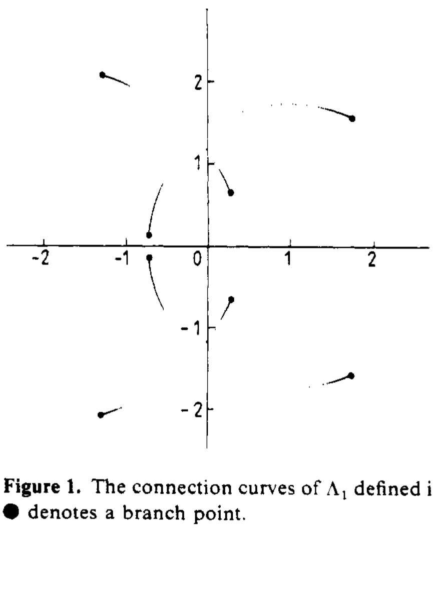


Figure 1. The connection curves of Λ_1 defined in (28) for the case $q=3$ in the $z=e^K$ place; ● denotes a branch point.

arcs lying mainly in the left half plane connect the points given by (31) and are not circular. The branch points in (3) occur at

$$\theta = \alpha \pm \pi/3 \qquad \left(\cos\alpha = \frac{1}{\sqrt{q}}, q>1\right) \tag{32}$$

and so the arcs on $|h|=1$ are of constant length $2\pi/3$.

For $m=3$ and $q=3$ τ_1 is a 3×3 matrix yielding a characteristic equation

$$\begin{aligned}\Lambda_1^3 - 9u^3(6\sqrt{3}w_2 + 10\sqrt{3} + 3w_3 + 16w_1)\Lambda_1^2 \\ + 27u^6(42\sqrt{3}w_3 + 287\sqrt{3}w_1 + 9w_4 + 252w_2 + 618)\Lambda_1 \\ - 81u^9(9\sqrt{3}w_4 + 324\sqrt{3}w_2 + 886\sqrt{3} + 114w_3 + 1200w_1) = 0\end{aligned} \tag{33}$$

where

$$w_j = u^j + u^{-j} \tag{34}$$

which again illustrates the symmetry represented by (26) and (27). On the real w_1 axis branch points of Λ_1^+ occur at $w_1 = 1.5194\ldots$ and $w_1 = -2.199\ldots$. The domain $|h|=1$ in (4) connects these two branch points by the real line segment between them; in the z plane this is the arc of the circle $1+\sqrt{3}\,e^{i\theta}$ shown in figure 2 and a real line segment connecting the points $z=-1.696\ldots$ and $z=-0.1127\ldots$. Figure 2 shows the connection curves C_3^{1+} for $|h|=1$; the extended system of connection curves is shown in figure 3 indicating the probable presence of structure in C_∞ additional to the circle $|u|=1$. An assessment of this additional structure awaits an extension of these calculations to larger values of m and will be reported elsewhere.

In a recent paper Martin (1986) obtains the partition function zeros of finite $m\times n$ lattices for the q-state Potts model. In the staggered ice model representation Martin shows that for $m\times\infty$ strips it is possible to confine the eigenvalues which are maximum in modulus to a single block of the transfer matrix and claims that finite lattice results can provide a good image of C_m. In the present context, when (and only when) such a factorisation is possible C_m will be a set of connection curves. Martin offers no explicit comparison of the finite lattice results with these curves. For example, in his figure 1 ($m=4$, $n=32$, $q=4$) the endpoints are claimed to be close to the branch

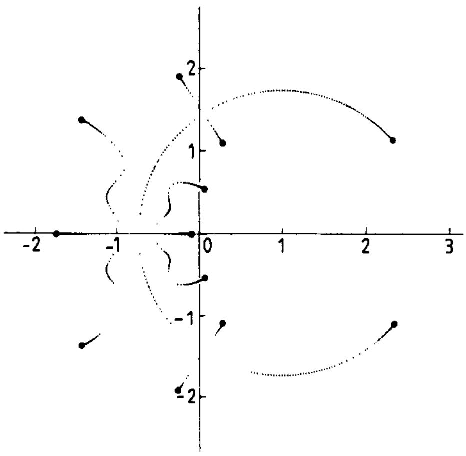


Figure 2. The connection curves C_3^{1+} in the $z=e^K$ plane obtained from (33); ● denotes the branch points of Λ_1^+.

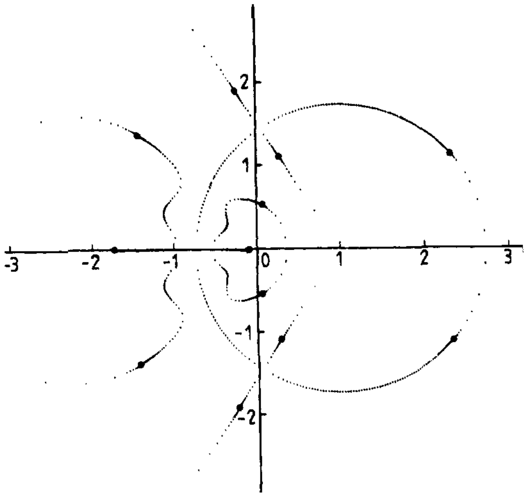


Figure 3. The extension of the connection curves in figure 2 in the domain of (4).

points of C_4, but the data reveal that there are 16 branch points and at most 12 endpoints. Presumably more structure is present in C_4 than is indicated in figure 1. The penultimate paragraph of Martin (1986) invites our comment. In the staggered ice representation the model loses the duality symmetry and (unlike C_m^{1+} above) the loci C_m do not contain arcs on $|u|=1$, for example C_4 extends to a very poor estimate of the critical point. The Ising model at $q=2$ is not a special case as is claimed.

For the triangular lattice with $m=2$ and a choice of the two boundary conditions shown in figure 4, referred to as (a) and (b), the characteristic equation of τ_1 is

$$\Lambda_1^2-[z^6+(2q-1)z^2+2(q-2)z+(q-2)^2]\Lambda_1+z^4(z-1)^2(z+q-1)=0 \tag{35}$$

for (a) or

$$\begin{aligned}\Lambda_1^2-[z^6+z^2(q+1)+4z(q-2)+(q-2)(q-3)]\Lambda_1\\ +z^2(z-1)^2[2z^4+4z^3(q-1)+z^2q(q-1)+(2z-1)(q-1)(q-2)]=0\end{aligned} \tag{36}$$

for (b).

The branch points of Λ_1^+ and the connection curves are given by (17) and the intersection points of the extended connection curves with the real axis are obtained

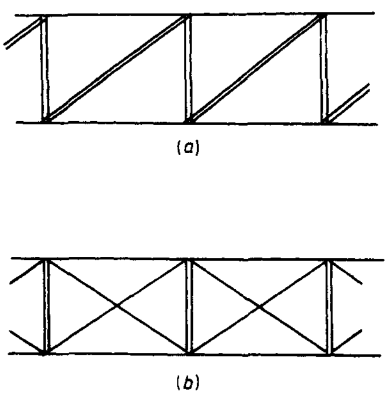


Figure 4. The boundary conditions (a) and (b) used to obtain Λ_1 in (35) and (36).

Table 1. The positive real axis intersection points of the extended connection curves of Λ_1 in (35) compared with the exact critical point of the Potts model on the triangular lattice.

q	1	2	3	4	5	6	7	8	9	10	50
z_c	1.5321	1.7321	1.8794	2.0000	2.1038	2.1958	2.2790	2.3553	2.4260	2.4920	3.9089
Intersection points	1.5000	1.7321	1.8966	2.0289	2.1416	2.2407	2.3298	2.4111	2.4862	2.5560	4.0254

from the roots of the equation

$$\mathrm{d}y/\mathrm{d}z = 0. \tag{37}$$

Those roots of (37) which form an approximation to the critical point are shown in table 1 for a range of q. For $q \geq 4$ and $q = 2$ the exact critical point is given by a root of the equation (Hintermann *et al* 1978)

$$\sqrt{q}u^3 + 3u^2 = 1. \tag{38}$$

It is generally accepted that (38) also holds for $q = 3$. The comparison of the real axis intersection points with the exact critical points in table 1 shows that they are encouragingly close approximations considering the low order of approximation at $m = 2$. The extended connection curves obtained from the roots of (17) for boundary conditions (a) and (b) are displayed in figures 5(a) and (b) respectively, and are superimposed in figure 5(c). Clearly the boundary conditions have had an effect (which we would expect to be maximal at $m = 2$), but even so the overall features are comparable and the closed curve in figure 5(a) is very closely followed by a combination of two of the branches of the resolvent (17). The extended connection curves for the case $q = 4$ in (36) are shown in figure 6; again the 'broad bean' shaped closed curve appears as the curve containing the critical point, which is at $z_c = 2$. The authors anticipate that these closed curves are already close to part of C_∞.

4. The Ising model on a non-planar lattice

Here we present an application of the present formalism to a two-dimensional Ising model on a non-planar lattice for which no exact information is available. The example chosen is a simple quadratic lattice with equal interactions between nearest-neighbour (NN) and next-nearest-neighbour (NNN) distances. The Hamiltonian is given by

$$-\beta H = K \sum_{\mathrm{NN}} \sigma_i \sigma_j + K \sum_{\mathrm{NNN}} \sigma_i \sigma_j. \tag{39}$$

Ising models which include an interaction range extending beyond nearest neighbours have been investigated by developing high- and low-temperature series expansions (Dalton and Wood 1969). For the present model the series expansion estimate for the critical point is

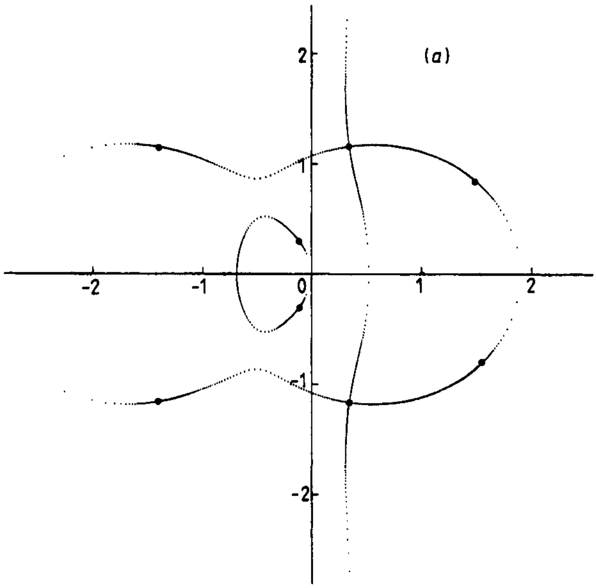
$$\mathrm{e}^{K_c} = 1.209. \tag{40}$$

For $m = 2$ and 3 the block τ_1 is quadratic and Λ_1 is defined by the equations

$$\Lambda_1^2 - \Lambda_1(z^3 + z + 2) + (z-1)^2(z^2 + 3z + 1) = 0 \qquad (m = 2) \tag{41}$$

and

$$\Lambda_1^2 - \Lambda_1(z^9 + 3z^3 + 3z^2 + 1) + 3z^2[(z^9 + 1)(z + 1) - z^2(z^3 + 1)^2] = 0 \qquad (m = 3) \tag{42}$$



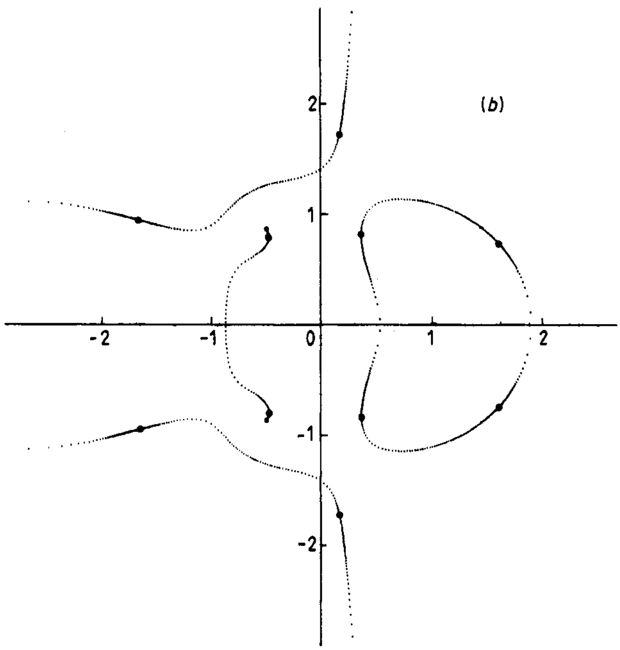


Figure 5. (a) and (b) are the extended connection curves of Λ_1 in (35) and (36) respectively for the case $q = 3$, in the $z = e^K$ plane; ● denotes the branch points. In (c), (a) and (b) are superimposed.

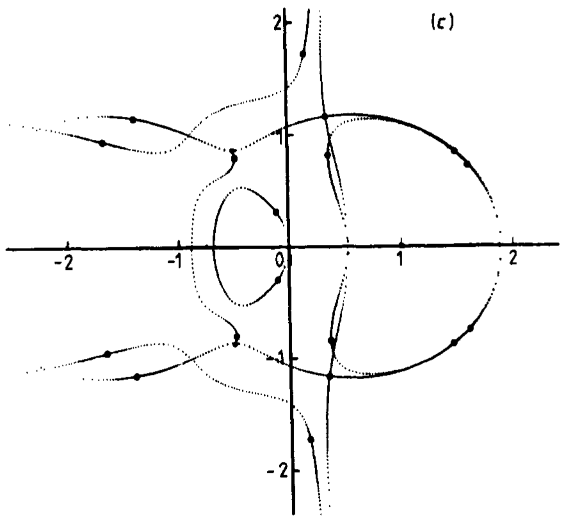


Figure 5. (continued)

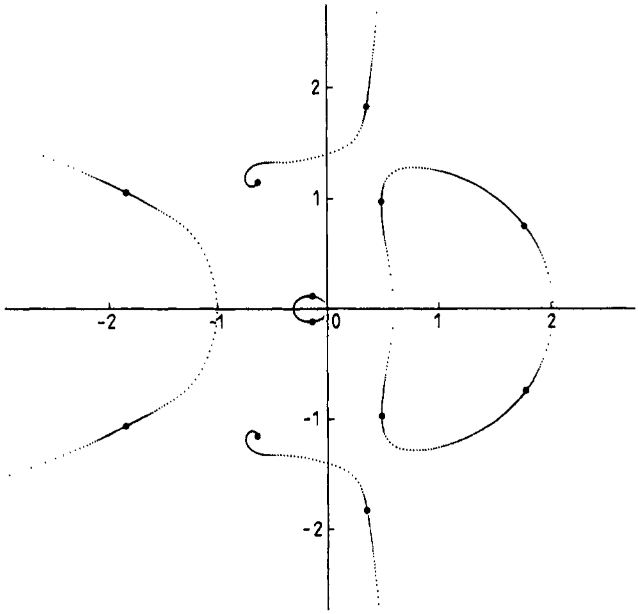


Figure 6. The extended connection curves of Λ_1 in (36) for the case $q=4$ in the $z=e^K$ plane; the exact critical point is at $z=2$ and the curve intersects the real axis at $z=2.0207\ldots$.

where $z=e^{4K}$. For $m=4$, Λ_1 is a four-valued function defined by the characteristic equation of τ_1 which is

$$\tau_1(z)=\begin{pmatrix} 2z^4c_{12} & 4z^2 & 8z^2c_6 & 2 \\ 2z^2 & 2c_4+2 & 8c_2 & 2z^{-2} \\ 2z^2c_6 & 4c_2 & 6c_4+2 & z^{-4}+1 \\ 2 & 4z^{-2} & 4z^{-4}+4 & z^{-8}+1 \end{pmatrix} \tag{43}$$

where $z=e^K$ and $c_n=\cosh nK$.

The connection curves of Λ_1 in (41) are C_2^{1+} and have been presented in figure 4(*b*) of I, and the curves in the extended domain of (4) are shown in figure 7 and are the branches $z_i(y)$ of the algebraic function

$$4y^2(z-1)^2(z^2+3z+1)=(z^3+z+2)^2 \qquad y \text{ real, } z=e^{4K} \tag{44}$$

(see (17)). The intersection with the positive axis occurs at

$$e^K = 1.241\ldots \tag{45}$$

which is already quite close to the critical point (40). At $m=3$, although the function Λ_1 is still only two valued the number of branch points increases. The system of connection curves over all of the branch points is shown in figure 8. In the extended domain of (4), these are the algebraic curves $z_i(y)$ defined by

$$12y^2z^2[(z^9+1)(z+1)-z^2(z^3+1)^2]=(z^9+3z^3+3z^2+1)^2 \qquad (z=e^{4K}). \tag{46}$$

The feature of particular interest is the 'near' overlapping arcs in the right half plane

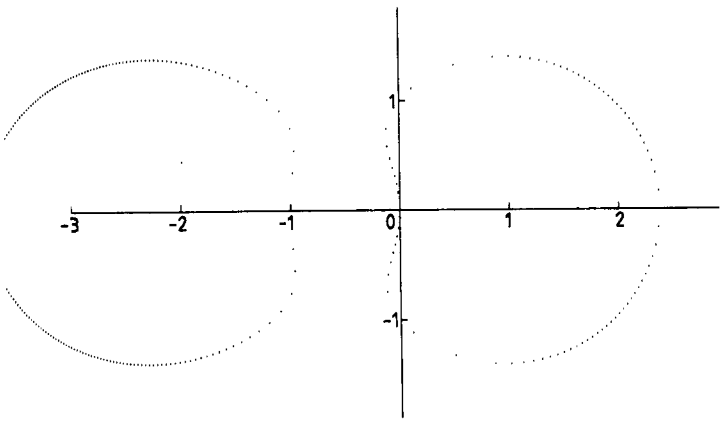


Figure 7. The extended connection curves of Λ_1 in (41) in the $z=e^{4K}$ plane; ● denotes the branch points.

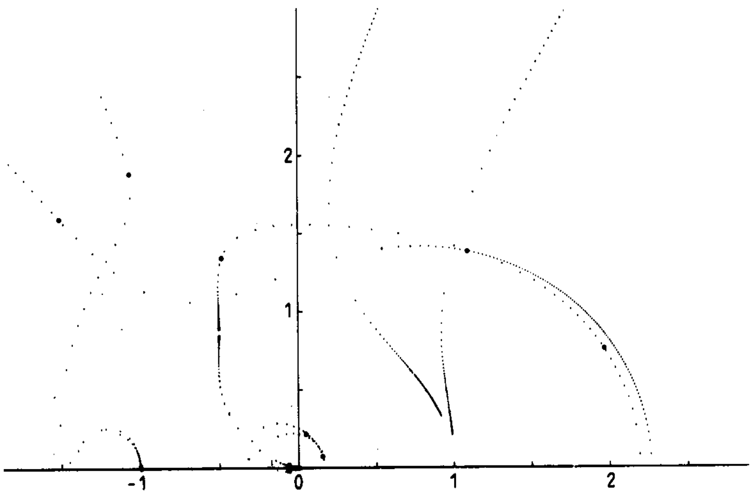


Figure 8. The extended connection curves of Λ_1 in (42) in the $z=e^{4K}$ plane; ● denotes the branch points.

in the approach to the real positive axis. The appearance of a closed curve which intersects the positive real axis is a feature common to both $m=2$ and $m=3$. The branch points which lie on this curve in figure 8 ($m=3$) generate the closed curve in the extended domain (4); the intersection with the positive axis occurs at

$$e^{K}=1.217\ldots \tag{47}$$

with a corresponding value of 1.23 from the 'near' overlapping arc.

At $m=4$, Λ_1 defined by the characteristic equation of (43) has 58 branch points, those lying in the complex plane being shown in the complicated system of connection curves shown in figure 9. Those branch points not on C_4^{1+} can be eliminated by

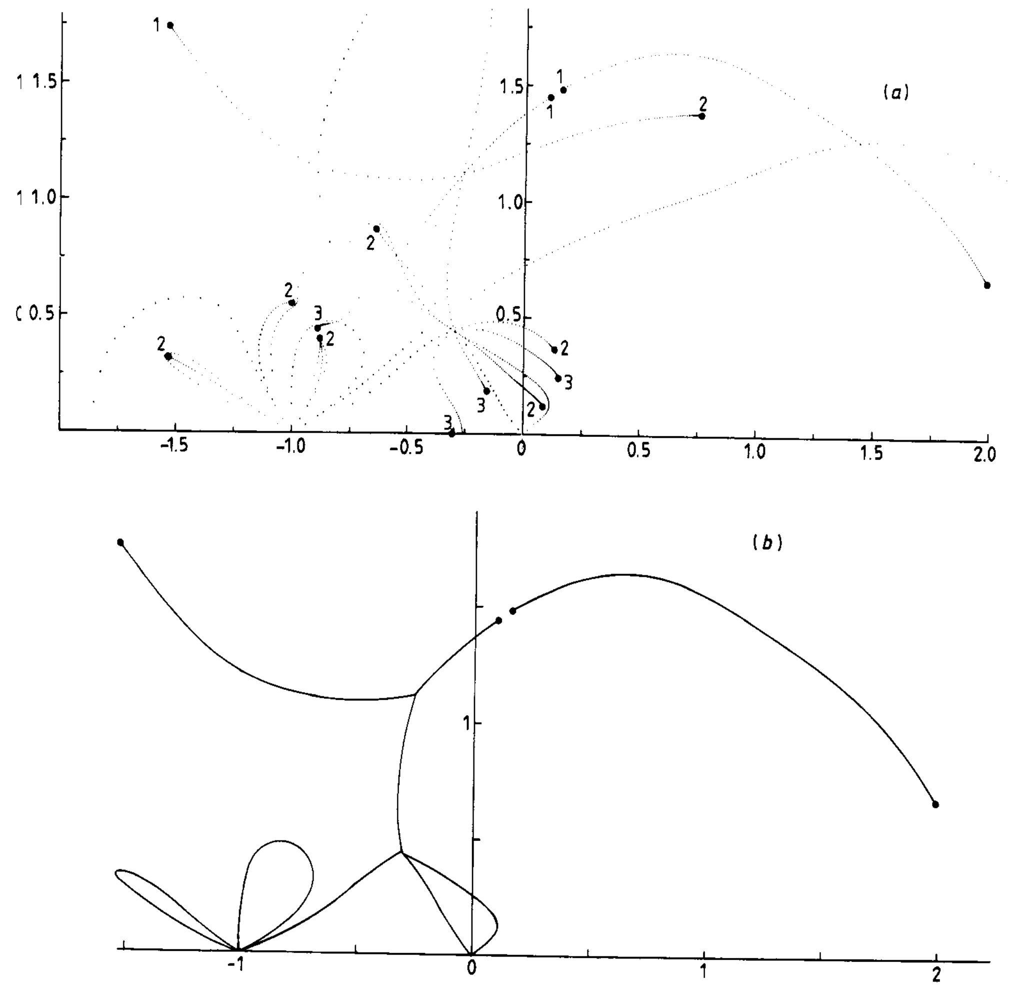


Figure 9. (*a*) The complex branch points and connection curves of Λ_1 defined by the characteristic equation of τ_1 in (43) in the $z=e^{4K}$ plane. The branch points ● are labelled 1, 2 or 3 according to the equal roots being maximum, second maximum, or smallest in modulus. Only four complex branch points are labelled 1 and only these lie on C_4^{1+}. (*b*) The extended connection curve C_4^{1+} abstracted from the connection curves in (*a*). At all points on the curve the branches of Λ_1 which are equal in modulus are simultaneously maximum in modulus.

evaluating the four roots at each branch point. In figure 9(a) each branch point is labelled 1, 2 or 3 according to whether the roots which are equal are maximum, second maximum or smallest in modulus, respectively. The curve C_4^{1+} emerges from its branch points until an intersection point is reached where more than two roots are of equal modulus. The path which emerges from an intersection point must again be determined by a determination of the four values of Λ_1. The outcome in the present case is the curve shown in figure 9(b). More structure has developed in the neighbourhood of the origin, and the curve extending into the negative half plane is also a feature in figure 8 for the case $m=3$. The approximation to the critical point is

$$e^K = 1.2127\ldots \tag{48a}$$

and closer to the series estimate (40). A purely numerical treatment at $m=5$ yields the corresponding intersection point to be at

$$e^K = 1.2110\ldots. \tag{48b}$$

5. The two-dimensional spin-1 Ising model

Here we consider the nearest-neighbour spin-1 Ising model on the simple quadratic lattice where the Hamiltonian is

$$-\beta H = K \sum_{\mathrm{NN}} \sigma_i \sigma_j \tag{49}$$

and the spin variables σ_i take the values 1, 0 and -1. Ising models with spin values of 1 and $\frac{3}{2}$ have been studied using low-temperature series expansions by Fox and Gaunt (1970, 1972) and Fox and Guttmann (1972); their estimate for the critical temperature on the quadratic lattice is

$$e^{-K_c} = 0.5533 \pm 0.0012. \tag{50}$$

We have considered only the case $m=2$ where the branches of Λ_1 are the eigenvalues of

$$\tau_1 = \begin{pmatrix} 1+z^4 & 2 & 2(1+z^2) & z \\ 2 & 1+z^{-4} & 2(1+z^2) & z^{-1} \\ 1+z^2 & 1+z^{-2} & 2+z+z^{-1} & 1 \\ 2z & 2z^{-1} & 4 & 1 \end{pmatrix} \qquad (z=e^K) \tag{51}$$

defined by the equation

$$\Lambda_1^4 - (16c^4 - 16c^2 + 2c + 7)\Lambda_1^3 + 2(c-1)[16c^2(c+1)^2 - 12c - 7]\Lambda_1^2 \\ - 16(c-1)^2(4c^3 + 3c^2 + c + 1)\Lambda_1 + 32(c-1)^4(c+1) = 0 \tag{52}$$

where $c = \cosh K$. The connection curves of Λ_1 are shown in the c plane in figures 10(a) and (b), and the branch points are again labelled 1, 2 or 3 according to whether the branches of Λ_1 which are equal are maximum, second maximum or smallest in modulus, respectively. Those curves which form C_2^{1+} are shown by the full curves in figure 10. The extended connection curves in the domain of (4) are shown in figure 11; the extension of C_2^{1+} yields a single intersection point on the real positive axis at a point corresponding to

$$e^{-K} = 0.5195. \tag{53}$$

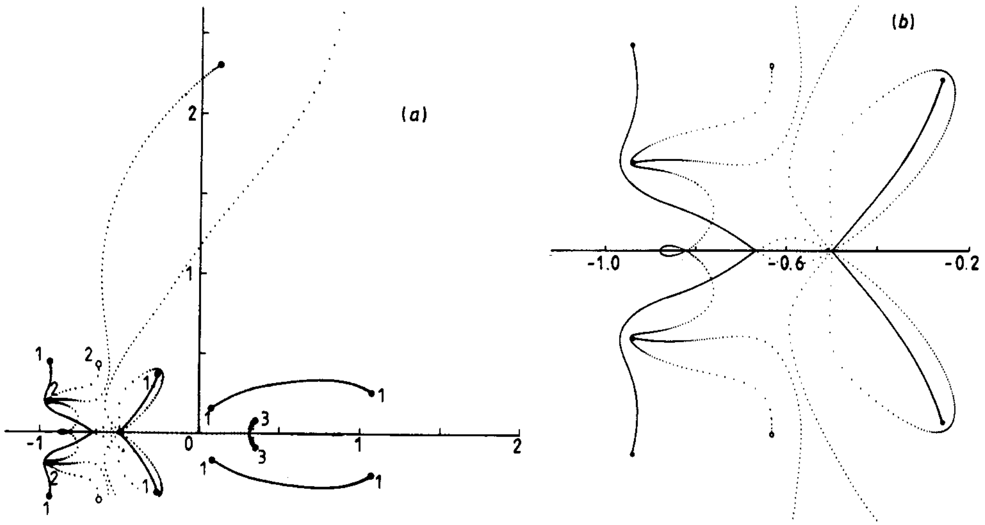


Figure 10. (a) The connection curves of Λ_1 in (52) in the cosh K plane. The branch points ● are labelled according to the scheme in figure 9(a). (b) A blow up of the connection curves in the neighbourhood of the negative axis. The curves which belong to C_2^{1+} are shown by the full curve.

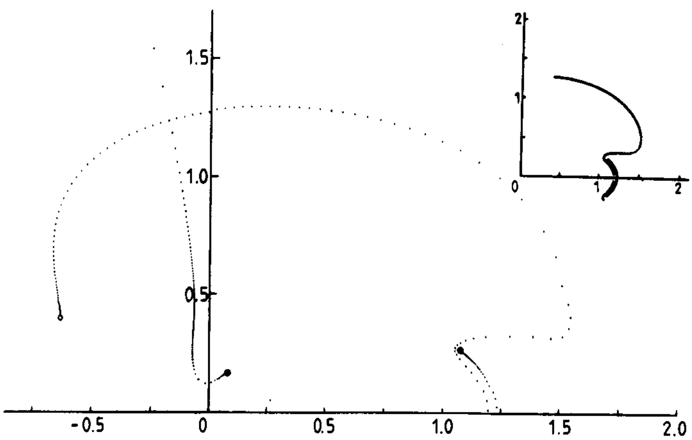


Figure 11. The extension of C_2^{1+} in figure 10 in the domain of (4) shown with an extension of a connection curve through the branch point denoted by ○ which does not belong to C_2^{1+}.

A striking feature of the extended connection curves is again the appearance of 'near' overlapping arcs in the vicinity of the critical point. In the present case however the arc lying close to C_2^{1+} is an extension of the curve through the branch point marked with an open circle in figure 11 which does not form part of C_2^{1+}; its intersection point with the real axis occurs at

$$e^{-K} = 0.555\ldots \tag{54}$$

which is very close to the critical point estimate (50). In § 3 it was observed that the duality symmetry for the spin-$\frac{1}{2}$ case on this lattice gave rise to branch points not connected by C_m^{1+} but which yielded extended connection curves overlapping C_m^{1+}. A similar phenomenon producing a 'near' overlap may have occurred in the present case with (54) viewed as a legitimate estimate of the critical point.

6. The three-dimensional Ising model

A very small scale application to the three-dimensional Ising model is possible in terms of the $2\times2\times\infty$ system which with full toroidal boundary conditions imposed is equivalent to a two-dimensional $2\times\infty$ system with anisotropic interactions in the ratio 1:2. It is thus possible to employ Onsager's solution to obtain the eigenvalues of the 16×16 transfer matrix in analytic form. The eigenvalue Λ_1^+ is given by

$$\Lambda_1^+ = 4\sinh^2 2K\, \mathrm{e}^{\gamma_1+\gamma_3} \tag{55}$$

where

$$\sinh 2K \cosh \gamma_1 = \cosh 4K \cosh 2K - \sinh 4K/(\sqrt{2}) \tag{56a}$$

and

$$\sinh 2K \cosh \gamma_3 = \cosh 4K \cosh 2K + \sinh 4K/(\sqrt{2}). \tag{56b}$$

The other branches of Λ_1 are given by (55) with exponents $-\gamma_1-\gamma_3$, $\gamma_3-\gamma_1$ and $\gamma_1-\gamma_3$. Using the latter pair of branches in conjunction with Λ_1^+ we can investigate the branch points and connection curves directly using equations of the type (7). We find that the connection curves are given by the branches $z(p)$ of two algebraic functions defined by

$$z^6 \pm \sqrt{2}z^5 + z^4(1-2p) + z^2(1+2p) \mp \sqrt{2}z + 1 = 0 \qquad p \text{ real},\ z = \mathrm{e}^{-2K}. \tag{57}$$

In (57) $|p|\leqslant 1$ corresponds to the domain $|h|=1$ in (4) and the branch points of Λ_1^+ occur at $p=\pm1$. If $z(p)$ are the branches of one of the equations (57) then the branches of the other are given by $z(-p)^{-1}$ and hence the branch points occur in reciprocal pairs. In fact both equations can be combined on multiplication into a single equation

$$u^6 - 4pu^5 + u^4(3+4p^2) + u^3(8-8p^2) + u^2(3+4p^2) + 4pu + 1 = 0 \tag{58}$$

where $u = \mathrm{e}^{-4K}$, which traces out all of these connection curves in the u plane. The branch points can be determined exactly; at $p=1$ (58) becomes

$$(u^2+1)(u^4-4u^3+6u^2+4u+1). \tag{59}$$

The roots of the quartic factor are of the form $r\mathrm{e}^{\pm i\theta}$ and $-(1/r)\mathrm{e}^{\pm i\theta}$, whence we find that

$$\cos^2\theta = (\sqrt{5}-1)/2 \tag{60}$$

and

$$r\cos\theta = 1 \pm (1+\cos^2\theta)^{1/2} \tag{61}$$

which in fact determines all of the branch points. These, together with the connection curves, are shown in figure 12(a), and the extended connection curves of the branch points at $u=\pm\mathrm{i}$ and those in the right half plane are shown in figure 12(b). The intersection points with the real positive axis can be determined from the roots of the equation

$$\mathrm{d}p/\mathrm{d}u = 0 \tag{62}$$

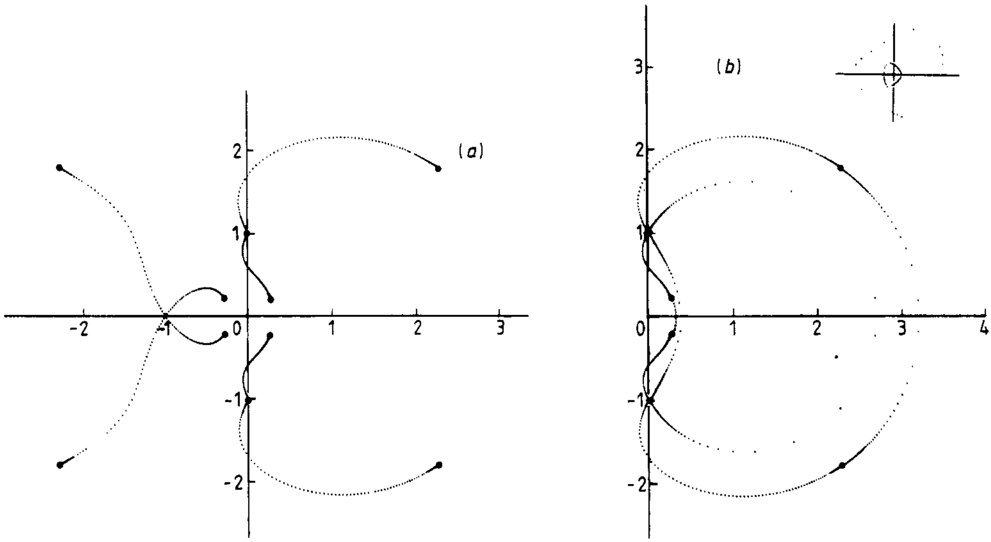


Figure 12. (a) The algebraic curves of (58) in the $u = e^{-4K}$ plane which are the connection curves involving Λ_1^+ for the smallest possible case of the three-dimensional Ising model on a $2\times2\times\infty$ strip; ● denotes the branch points. (b) The extended connection curves through the branch points at $u = \pm i$ and the pair in the right half plane. The zeros of the $4\times4\times4$ cube obtained by Pearson (1982) are shown in the inset for comparison.

which are those of the symmetric polynomial equation

$$2u^8-9u^7+6u^6-7u^5+48u^4-7u^3+6u^2-9u+2=0. \tag{63}$$

The real axis intersection points are

$$u=3.2007\ldots \qquad u=0.372\,49\ldots \tag{64a}$$

and

$$u=2.6846\ldots \qquad u=0.312\,42\ldots. \tag{64b}$$

The critical point estimate from series expansions is at $u=2.427\ldots$ and the critical point of the anisotropic 2D model is at $u=3.3829\ldots$. In figure 12(b) the zeros of the $4\times4\times4$ cube obtained by Pearson (1982) are shown for comparison.

7. Models with three-site interactions present

Here we consider examples of one-parameter models defined in terms of triplet interactions. Two generalised Potts models are of interest where the lattice is the triangular lattice and the interaction is scalar Potts-like over the three sites of each elementary triangle. The site variables σ_i take the values $1, 2, \ldots, q$ which can be viewed as colours. The reduced energy of any configuration of the lattice in units of K is simply equal to the number of triangles whose vertices are all the same colour. The two models in question are the cases where (a) the interactions are defined over only half of the triangles (the up pointing triangles say) of the lattice, and (b) the interactions are defined over all of the triangles. Baxter *et al* (1978) have derived a duality relation for model (*a*) (including the case where Potts pair interactions are also present) which for triplet interactions only can be expressed in the form

$$w^{-N/2}Z_N(q, w) = w^{N/2}Z_N(q, w^{-1}) \tag{65}$$

where

$$w = (z-1)/q \qquad z = \mathrm{e}^K. \tag{66}$$

The argument following (24) for the Potts models can now be applied here and the characteristic equation of τ_1 can be mapped out in terms of reduced polynomials of the type defined in (27) with u replaced by w; hence the extended connection curves for any value of m include the circle $|w| = 1$. It is known rigorously (Wu and Zia 1981) that for $q = 2$ and $q \geq 4$ the critical point is the point $w = 1$. The argument here shows that C_m^{1+} for all m includes arcs of the circle $|w| = 1$. This symmetry is already evident at $m = 2$ where

$$\Lambda_1^2 - (z^2+8)\Lambda_1 + 4(z-1)^2 = 0 \qquad z = \mathrm{e}^K \tag{67}$$

which on writing $\Lambda_1 = qwy$ yields the reduced equation

$$y^2 + [q(w+w^{-1})+2]y + (q-1)^2 = 0 \tag{68}$$

showing that Λ_1^+ has branch points at $w = \mathrm{e}^{\mathrm{i}\theta}$ where

$$\cos\theta = 1 - 2/q \quad \text{and} \quad \pi \tag{69}$$

which are connected on $|w| = 1$.

For case (*b*) above no duality relation exists. For $m = 2$ Λ_1 is given exactly by (67) with z replaced by z^2. Thus the extended connection curve is the circle

$$z^2 = 1 + q\,\mathrm{e}^{\mathrm{i}\theta} \tag{70}$$

indicating an approximation to the critical point for $q = 3$ of $\mathrm{e}^{-K} = \frac{1}{2}$. Enting and Wu (1982) have developed low-temperature series expansions for this model in the special case of $q = 3$. On the basis of a low-temperature expansion of the order parameter up to terms of order 33 in the variable e^{-K} these authors obtained the critical point estimate

$$\mathrm{e}^{-K_c} = 0.5038 \pm 0.0005 \tag{71}$$

and therefore the estimate of $\frac{1}{2}$ obtained from (70) is apparently already very close to the critical point. At $m = 3$ (and $q = 3$) τ_1 is the matrix

$$\tau_1 = \begin{pmatrix} z^6+2 & 6(z^3+z+1) & 6z \\ z^3+z+1 & 4z^2+2z+12 & 2z+4 \\ 3z & 6(z+2) & 6 \end{pmatrix} \qquad z = \mathrm{e}^K. \tag{72}$$

Figure 13 shows C_3^{1+} compared with the circle (70) which is C_2^{1+} in the z^2 plane. The intersection of the extension of C_3^{1+} with the real axis occurs at

$$\mathrm{e}^{-K} = 0.509\,28\ldots. \tag{73}$$

The three-spin Ising model on the triangular lattice (Baxter and Wu 1974, Baxter 1974, §§ 2 and 5 of I) possesses a self-dual symmetry of precisely the same type as the two-dimensional Ising model (Wood and Griffiths 1972, Merlini and Gruber 1972) with a dual temperature K^* defined by

$$ss^* = 1 \qquad s = \sinh 2K. \tag{74}$$

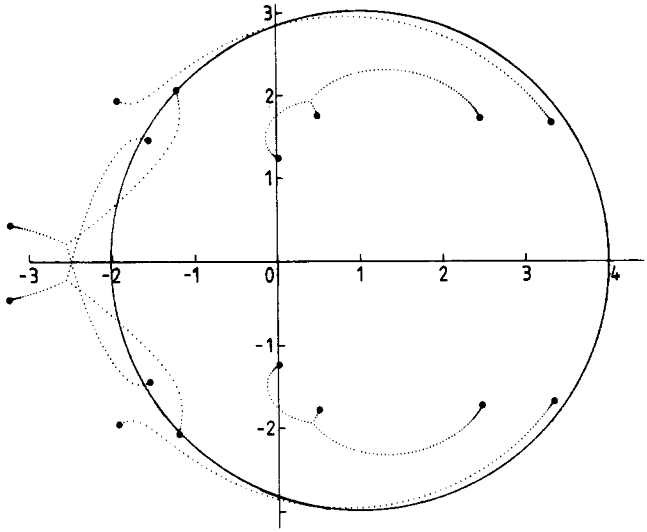


Figure 13. The connection curves which form C_3^{1+} of Λ_1 (shown dotted) defined by (72) in the $z^2 = e^{2K}$ plane. The extended connection curve C_2^{1+} is the circle (70) with $q = 3$ shown by the full curve. The extension of C_3^{1+} intersects the real axis at $z^{-1} = 0.509\,28\ldots$, and the series estimate for the critical point is $z_c^{-1} = 0.5038 \pm 0.0005$.

The previous arguments can again be carried through to infer that the characteristic equation of τ_1 for any value of m can be mapped out in terms of reduced polynomials of the type defined in (27) with u replaced by s, and the circle $|s| = 1$ appears as part of the extended connection curves C_m^{1+} for all m. For example at $m = 3$ with toroidal boundary conditions

$$\tau_1 = \begin{pmatrix} 3z^2 + z^{-6} & 4 \\ 4 & 3z^{-2} + z^6 \end{pmatrix} \tag{75}$$

and writing

$$\Lambda_1 = \tfrac{1}{2} \sinh 4K\lambda \tag{76}$$

$$\lambda^2 - 8(s + s^{-1})\lambda + 48 = 0 \tag{77}$$

where λ has a branch point at $s = e^{i\theta}$, $\cos\theta = \pm\sqrt{3}/2$. Again using screw boundary conditions (Wood and Griffiths 1972) with a screw pitch of 3, the 8×8 transfer matrix yields a characteristic equation

$$\lambda^2(\lambda^6 - 2\cosh 2K\lambda^5 + 16 \sinh^2 2K \cosh^2 2K) = 0 \tag{78}$$

which on writing $\lambda = 2\cosh 2Ky$ yields the factor

$$y^6 - y^5 + \tfrac{1}{4}(s + s^{-1})^{-2} = 0. \tag{79}$$

Λ_1^+ has branch points at $s = e^{i\theta}$ where

$$\cos^2\theta = \tfrac{3}{8}(\tfrac{6}{5})^5 \tag{80}$$

and $|s| = 1$ is the extended connection curve obtained from (78) (see figure 7 of I).

8. The Ising model in a field

Within the formalism of the present work we briefly consider the original theorem of Lee and Yang (1952) and its extension to the general spin model by Griffiths (1969). In this we now consider a many-parameter model mapped out in terms of a set of temperature variables $z\{z_i = e^{K_i}\}$ and a field variable $\mu = e^{\beta H}$, where K_i is the interaction parameter over a range of type i. Following the notation of Griffiths (1969) the Ising-model spin variables take the values $p, p-2, p-4, \ldots, 2-p, -p$, corresponding to a spin of $p/2$. The partition function for any arbitrary system of N spins can be written in the form of a symmetric polynomial in the variable μ^2:

$$Z_N = \mu^{-Np} \sum_{k=0}^{Np} A_k(z)\mu^{2Np-2k} \tag{81}$$

where $A_k(z)$ are positive temperature-dependent coefficients and $A_k = A_{Np-k}$. The theorems of Lee and Yang (1952) and Griffiths (1969) state that for ferromagnetic interactions ($K_i > 0$) and at real values of z the zeros of (81) all lie on the unit circle $|\mu| = 1$ (see also Ruelle 1969). In the limit of $N \to \infty$ one envisages that the zeros of (81) become dense over parts of the unit circle $|\mu| = 1$.

In the present work we are in fact concerned with the limit of $N \to \infty$ in the limiting locus C_m for a semi-infinite regular lattice on which a transfer matrix T_Ω can be defined. For any such general spin Ising model the transformation $\mu \to \mu^{-1}$ is simply equivalent to a re-ordering of the basis of T_Ω. Hence the whole of the characteristic equation of T_Ω can be mapped out in terms of the variables z and $w = \mu + \mu^{-1}$. Thus at real temperatures and $|\mu| = 1$ or μ real the eigenvalues of T_Ω are either real or in complex conjugate pairs, and the extended connection curves in the domain of (4) map out the circle $|\mu| = 1$ for all m. The branch points of Λ_1 are given by the resolvent (20) of I which at $h = 1$ is now a polynomial in w with coefficients which are multinomials in the temperature variables z. The algebraic functions $w_i(z)$ defined by this resolvent at $h = 1$ denote the location of the branch points as the temperature varies, and for real w the branch points in the μ plane lie on either the real axis or the unit circle. The eigenvalue Λ_1^+ cannot have any branch points on the real axis of μ at finite values of z. This follows from the form of T_Ω which can always be written in the form

$$T_\Omega = \mu^{-Np} T'_\Omega(z, \mu^2). \tag{82}$$

T' is a strictly positive matrix everywhere on the real axis of μ. Hence in the domain of real w for finite z, if Λ_1^+ has any branch points they must lie on the circle $|\mu| = 1$. Thus we expect Λ_1^+ to possess algebraic singular points on the unit circle whose location is temperature dependent. In the trivial example of the one-dimensional nearest-neighbour model ($p = 1$) Λ_1^+ has a branch point at $\mu = e^{i\theta}$ where

$$\sin\theta = \pm z^{-2} \qquad (z = e^K) \tag{83}$$

which in the limit of zero temperature occurs at $\mu = \pm 1$, and in the limit of infinite temperature at $\mu = \pm i$. Similar limits occur in nearest-neighbour models generally, since if we consider the limit

$$\lim_{z\to\infty} \lambda_i / z^s \qquad i = 1, 2, \ldots, \Omega \tag{84}$$

where s is the total number of nearest-neighbour pairs in G and connecting G_1 and

G_2 (see § 2 of I) and λ_i are the eigenvalues of T_Ω, we obtain

$$\lim_{z\to\infty} \frac{\lambda_i}{z^s} = \begin{cases} \mu^{mp} & i=1 \\ \mu^{-mp} & i=2 \\ 0 & i=3,\ldots,\Omega \end{cases} \tag{85}$$

and

$$\lim_{z\to\infty} \lambda_1/\lambda_2 = \mu^{2mp}. \tag{86}$$

Hence the $2mp$ roots of unity are limiting branch points of Λ_1^+ in the limit of $T \to 0$. Again in the limit of $z \to 1$

$$\begin{aligned} &\Lambda_1^+ = (\mu^p + \mu^{p-2} + \ldots + \mu^{-p})^m \\ &\lambda_i = 0 \qquad i = 2,\ldots,\Omega \end{aligned} \tag{87}$$

and thus Λ_1^+ has limiting branch points at $\mu = \pm e^{i\theta/2}$ when $e^{i\theta}$ are the p complex roots of the $(p+1)$th roots of unity. We are thus led to expect that in the range $1 < z < \infty$ branch points of Λ_1^+ will lie on the unit circle, and that in the limit of $m \to \infty$ the singular points of the limiting partition function per site Λ will evolve through a sequence of algebraic singular points. At $T = T_c$ we expect branch points on $|\mu| = 1$ to approach the limit $\mu = 1$ in the limit of $m \to \infty$.

9. The hard square and hard hexagon lattice gases and the q colourings of the triangular lattice

The nearest-neighbour hard core lattice-gas models are models in which the atoms are prohibited from simultaneously occupying nearest-neighbour (NN) sites by an infinite repulsive short-range interaction. If t_i are the site variables with the values $t_i = 1$ and 0 denoting an occupancy and a vacancy, respectively, of site i, then the grand canonical partition function Ξ for any such lattice model can be written as

$$\Xi_N(z) = \sum_{\{t\}} \prod_{\mathrm{NN}} (1 - t_i t_j) \prod_{i=1}^{N} z^{t_i} \tag{88}$$

where z is the activity variable. The hard square gas on the simple quadratic lattice has been studied by numerous authors (Gaunt and Fisher 1965, Ree and Chestnut 1966, Runnels and Combs 1966, Runnels 1972, Nilsen and Hemmer 1967, Baxter *et al* 1980, Wood and Goldfinch 1980). For the hard hexagon gas on the triangular lattice the partition function (88) has been obtained exactly in the thermodynamic limit by Baxter (1982). Here we consider the present formalism applied to both of these models.

The work of Nilsen and Hemmer (1967) also considered the location of the partition function zeros in the z plane for semi-infinite strips in the hard square gas case but with non-toroidal boundary conditions which allowed a one-dimensional representation of the problem. These authors developed a formalism which employed the seldom used grand pressure ensemble and C_m is obtained from the z-dependent residues of the poles of the grand pressure partition function. In this, some similarities with the present work can be seen in which C_m is obtained as a subset of trajectories in the z plane over which the residues are of equal modulus. Nilsen and Hemmer employed their method to obtain an estimate of the singularity in the limiting partition function per site on the negative real axis.

In the present work the algebraic functions Λ_1 for the hard square gas and $m=2$, 4 and 6, respectively, are defined by the equations

$$m=2 \qquad \Lambda_1^2-\Lambda_1(z+1)-z=0 \tag{89}$$

$$m=4 \qquad \Lambda_1^3-\Lambda_1^2(z^2+3z+1)+\Lambda_1 z(z^2-z-1)+z^3=0 \tag{90}$$

$$\begin{aligned} m=6 \qquad & \Lambda_1^5-\Lambda_1^4(z^3+5z^2+5z+1)+\Lambda_1^3 z(2z^4+6z^3-4z-1) \\ & +\Lambda_1^2 z^3(2z^4+5z^3+9z^2+7z+2)+\Lambda_1 z^5(2z^3+2z^2-z-1)-z^8=0 \end{aligned} \tag{91}$$

and for the hard hexagon gas with $m=3$ and 6

$$m=3 \qquad \Lambda_1^2-\Lambda_1(1+z)-2z=0 \tag{92}$$

$$\begin{aligned} m=6 \qquad & \Lambda_1^5-\Lambda_1^4(z^2+4z+1)-2\Lambda_1^3 z(2z^4+4z+1)+2\Lambda_1^2 z^3(3z^2+7z+4) \\ & +4\Lambda_1 z^5(z-1)-8z^8=0. \end{aligned} \tag{93}$$

In figures 14–16, we show the connection curves of C_m^{1+} for (90), (91) and (93), respectively, extended in the domain of (4). For the hard square gas the intersections with the positive z axis occur at 3.016... ($m=4$) and 3.730... ($m=6$); the most reliable estimate of z_i is 3.796 obtained from the low-density expansions of Baxter *et al* (1980). In figure 16 the intersection point occurs at $z=11.445\ldots$ and the exact critical point is $z_c=(11+5\surd5)/2=11.090\ldots$.

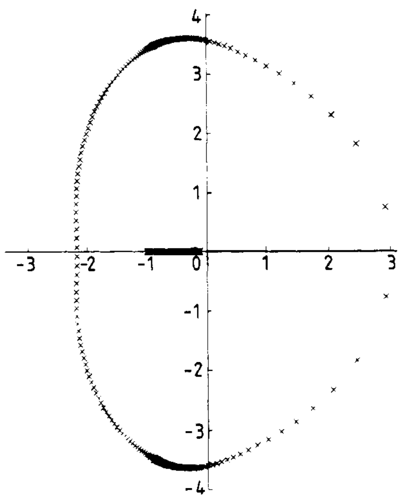


Figure 14. The hard square gas: the extended connection curves of Λ_1 ($m=4$) of (90) in the z plane.

In all of the examples of Λ_1 above branch points occur on the negative real axis and the domain $|h|=1$ in (4) traces out a system of connection curves along the real negative axis which connect up these branch points. Viewed over a sequence of increasing m these represent a sequence of overlapping line elements converging to a part of C_∞ which is the line element on the negative real axis with an endpoint close to the origin where the limiting partition function per site is singular. For the hard hexagon model (92) and (93) yield branch points at $-5+2\surd6=-0.101\,02\ldots$ and $-0.093\,77\ldots$, respectively. The singularity in the thermodynamic limit is at $z=(11-5\surd5)/2=0.090\,169\ldots$ (Baxter 1982). For the hard square gas the corresponding

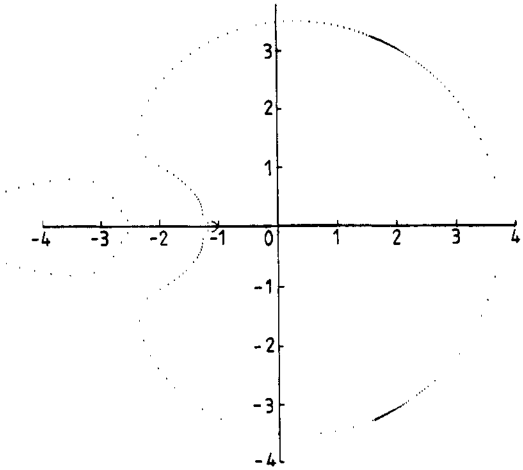


Figure 15. The hard square gas: the extended connection curves of Λ_1 ($m=6$) of (91) in the z plane. The real positive axis intersection point is at $z=3.730\ldots$, and the series estimate for z_c is $3.796\ldots$.

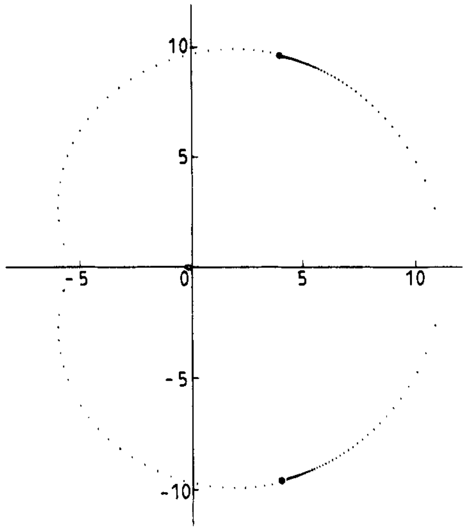


Figure 16. The hard hexagon gas: the extended connection curves of Λ_1 ($m=6$) in (93) in the z plane. The real positive intersection point is at $z=11.44\ldots$, and the critical point z_c is $11.090\ldots$.

branch points move smoothly from $z=-3+2\surd 2=-0.171\,57\ldots$ at $m=2$ to $z=-0.119\,496\ldots$ at $m=13$. A similar sequence was obtained by Nilsen and Hemmer (1967). In an initial investigation of the present techniques using the hard square gas model one of us (Wood 1985) considered the transformation

$$\Lambda_1=\lambda+(1/r)\,\mathrm{Tr}\,\tau_1 \tag{94}$$

where r is the dimensionality of τ_1. On an examination of the connection curves of λ^+ for the case $m=4$ in the domain $|h|=1$ only, an intersection point on the real

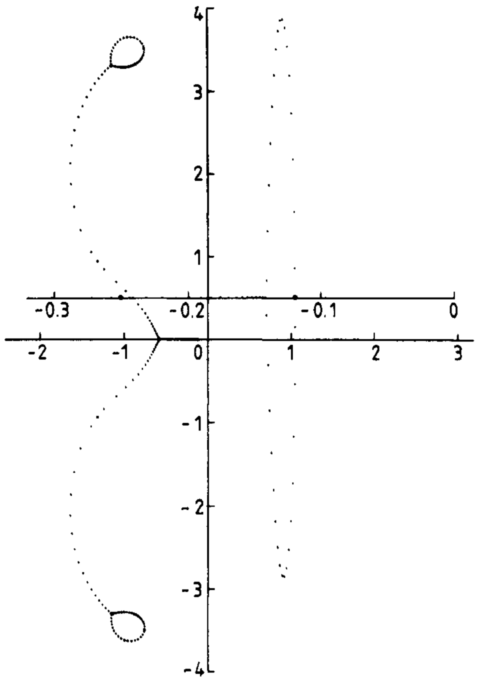


Figure 17. The connection curves of λ in (94) where Λ_1 is given by (90) and the intersection point with the real axis beyond the branch point is at $x = -0.119\,392\ldots$.

negative axis occurs at $z = -0.119\,392\ldots$. These curves are shown in figure 17 in which the connection between the branch points on the negative axis becomes extended by the tiny loop element shown in the inset of figure 17. This behaviour and the comparison with the series estimate of $z = -0.1194 \pm 0.0002$ obtained by Gaunt and Fisher (1965) for the real negative singularity tempted the conjecture that the above result may be exact. This is not the case and estimates of this singularity have now been improved to

$$z = -0.119\,338\,8809 \pm 0.000\,000\,001 \tag{95}$$

by Guttmann (1987) and Dhar (1986).

Baxter (1986) has recently obtained exactly the chromatic polynomial of the plane triangular lattice in the thermodynamic limit. This model is obtained as the zero-temperature limit of the antiferromagnetic q-state Potts model in which the only lattice configurations which can occur are those in which the vertices of each elementary triangle are in different states. Alternatively the model can be viewed as a hard core model of a gas of q components or colours for which nearest-neighbour exclusion applies to atoms of the same type. For $m = 4$ and arbitrary q Λ_1 is the two-valued function given by

$$\Lambda_1^2 - \Lambda_1 u(u^3 + 6u - 3) + 2u^3(u^3 + 2u^2 - 1) = 0 \tag{96}$$

where $u = q - 3$. For this model the transfer matrix and τ_1 are positive matrices for $q > 4$ and Λ_1 in (96) has a real branch point at $q = 4$. Baxter has also obtained the locus of zeros of the chromatic polynomial C_∞ which in figure 18 is compared with

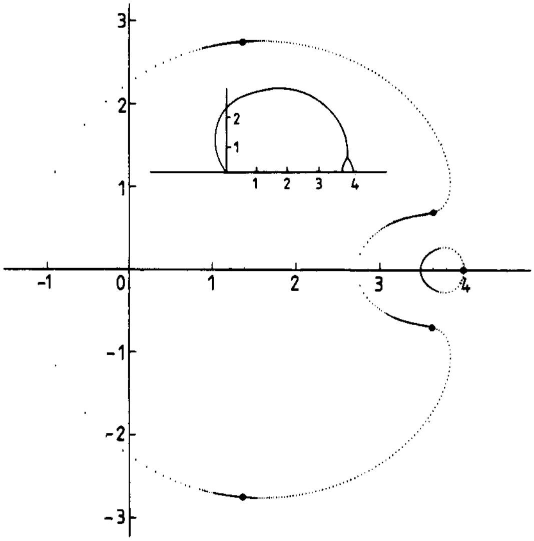


Figure 18. The extended connection curves of Λ_1 of (95) in the q plane; C_∞ is the full curve obtained by Baxter (1986).

the connection curves C_4^{1+} of (96) in the domain of (4)†. The branch points are marked by full circles. The curves C_4^{1+} represent the lowest order of approximation in this case and the real axis point $q=4$ has emerged exactly. In addition, C_4^{1+} appears to have given a faithful representation of the overall structure of C_∞. An investigation of C_8^{1+} would be of great interest here.

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† The full curve sketched in figure 18 misrepresents the intersection at $q=4$ which is a cusp (see Baxter 1987).

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