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On a Point of Order

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A method of using algebraic curves to obtain estimates of critical points accurate enough to identify them as simple algebraic numbers (if that is what they are) is discussed and illustrated with an application to the q-state Potts model on the triangular lattice for cases of pure two-site interactions and pure three-site interactions. In the latter case the critical point is conjectured to be $z_c^2 = (\frac{1}{2}\sqrt{3})^{(q-2)/2} + q$ $(q \geqslant 1)$. In a similar conjecture for the critical percolation probability on the *directed* square lattice, $q_c^{1/2}(q_c + 3) = 2$ $(q_c + p_c = 1)$.

KEY WORDS: Statistical mechanics; Potts models; algebraic functions; transfer matrix.

1. INTRODUCTION

The occasion to reminisce seldom presents itself in the scientific text; perhaps a brief indulgence is possible (D.W.W.). Below spring tide level in the gloomy depths of the Wheatstone Laboratory (reconstructed from a cavity in part created by the Luftwaffe) graduate students relinquished their remaining hold on innocence. Spin Hamiltonians, power series, embeddings, confidence limits (!), and double length arithmetic "close in on the growing boy."[(1)] The demands of eyeball counting were heavy; few escaped with an eyesight unimpaired. In the years following their experiences at King's College London many continued to find much to interest them in the continuing growth and development of lattice models in statistical mechanics.

In 1965 at a conference on critical phenomena in Washington, Domb[(2)] speculated on the possibility of engineering exact solutions to critical phenomena. The approach was combinatorial and considered the asymptotic growth of the embeddings of classes of multiply connected

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graphs which contribute to terms in the high-temperature power series expansions found in the Ising model. A difficult problem in itself, but one considered to be simpler than the Ising problem. In this paper we adopt the engineering spirit and present a novel and hopefully even an entertaining method of "guessing" exact critical points. In this approach the emphasis is focused upon the transformation structure that can be found in the algebraic functions generated by finite transfer matrices. The guessing game is *not* simply on grounds of numerical extrapolation; very accurate numerical data are indeed obtainable, but alongside is the search for evidence of a transformation symmetry analogous to the simple inversion symmetry of the self-duality transformation, but which may only become exact asymptotically (with fixed boundary conditions).

Guessing sets of rational fractions for exponents on the basis of data gleamed from expansions was (and still is) a popular pastime, but much less so for critical points. The critical points which are known exactly are simple algebraic numbers, where simple means polynomials of low degree and very small integer coefficients. Thus, Gaunt, using data obtained from low- and high-density expansions of only modest accuracy, correctly guessed

$$z^2 - 11z - 1 = 0 \tag{1}$$

for the singularities of the grand canonical partition function of the hard-hexagon model, where z is the activity (Baxter[3]). It has been shown recently[4] that (1) can be inferred "exactly" in a technique similar to those described here. In Section 2 we discuss sequences of algebraic curves and algebraic branch points which can respectiyely throw some light on close algebraic symmetry and form very accurate numerical estimates of critical points. In Section 3 we illustrate both of these features in applications to both the two-site and three-site q-state Potts model on the triangular lattice, and in the declared spirit present a conjecture that the critical point of the three-site model is given by

$$z_c^2 = \left(\frac{\sqrt{3}}{2}\right)^{(q-2)/2} + q \qquad (q \geqslant 1) \tag{2}$$

A conjecture for p_c in the directed percolation problem on the square lattice is also added.

Although in this paper we concern ourselves only with the critical point, numerical estimates of leading exponents in the *partition function* at its singular points (both physical and nonphysical) can be extracted from sequences of algebraic branch points in the complex temperature plane. Details of this and other aspects will appear in future publications.

2. CIRCLES, ALMOST CIRCLES, AND BRANCH POINTS

Following recent work,[4-9] we are concerned with certain algebraic functions generated by a finite transfer matrix. Here our examples are all two dimensional, where $T_m(z)$ denotes the transfer matrix of an $m \times n$ strip. The single variable z (we consider a one-parameter model) is a suitable temperature variable and the elements of $T_m(z)$ are arranged to be positive integer powers of z. The transfer matrix is reduced to block diagonal form

$$T_m(z) = \bigoplus_k \tau_k(z) \tag{3}$$

such that each $\tau_k(z)$ whose elements are polynomials in z is *irreducible*. Taking $\tau_1(z)$ to be the symmetric block, then the characteristic equation of $\tau_1(z)$ defines an irreducible algebraic equation

$$F(\Lambda, z) = \sum_{\alpha\beta} A_{\alpha\beta} \Lambda^\alpha z^\beta = 0 \qquad (A_{\alpha\beta} \text{ integer}) \tag{4}$$

and a single algebraic function Λ, one of the function elements of which Λ_1^+ is the partition function per site of the $m \times \infty$ strip $(z > 0)$.

We can view the function

$$Z_{mn}^{(1)}(z) = \text{Trace } \tau_1^n(z) \tag{5}$$

as a block partition function which becomes the partition function per site in the limit of $n \to \infty$ on the nth root of $Z_{mn}^{(1)}$. The zeros of the block partition function in the limit of $n \to \infty$ lie in regions of the z plane where the eigenvalues of $\tau_1(z)$ are simultaneously equal and maximum in modulus. This region is necessarily an *algebraic curve* for m finite and is denoted by C_m^{1+}. The algebraic equation which will generate this curve is the resolvent polynomial between (4) and

$$F(\Lambda h, z) = 0 \tag{6}$$

which on allowing for trivial factors and the obvious inversion symmetry on $h \to h^{-1}$, can be expressed as a polynomial equation

$$R_m(w, z) = \sum_{\alpha\beta} C_{\alpha\beta} z^\alpha w^\beta \qquad (C_{\alpha\beta} \text{ integer}) \tag{7}$$

where $w = \frac{1}{2}(h + h^{-1})$. Thus, for real w on $|w| \leqslant 1$ the branches of (7) trace out a system of algebraic curves connecting the branch points of Λ. C_m^{1+} is the subset of these curves along which the eigenvalues which are equal in modulus are *simultaneously* maximum in modulus.

The branch points of Λ on C_m^{1+} are of special interest; they are given by (7) with $w=1$, which is the discriminant of (4). From this viewpoint the mechanism by which a real critical point z_c emerges in the full thermodynamic limit of $m \to \infty$ is algebraic in that the algebraic singular points of $\Lambda_1^+(m, z)$ converge onto z_c. Simultaneously, the sequence C_m^{1+} converges onto the limiting locus of the block partition function zeros. The curve C_m^{1+} is naturally extended on the domain w real, $|w| > 1$. This extension through the end point of C_m^{1+} which is closest to the positive real axis extends the curve down to an intersection point $z_c(m)$ on the real axis which forms an approximation to the critical point. The extension of C_m^{1+} appears always to have quadratic curvature across the real positive axis, and in cases where C_∞^{1+} is orthogonal to the real axis at z_c the points $z_c(m)$ are frequently amazingly close to z_c (see Table I); this gives rise to an interesting problem. The resolvents (7) are both wonderously long and irreducible (trivial factors apart), even for small values of m. The integer coefficients become very large *very* rapidly, so how exactly does a simple algebraic factor such as (1) emerge in the limit of $m \to \infty$?

Figures 1 and 2 show C_7^{1+} for the 2-state Potts model (equivalent to the Ising model) on the triangular lattice; the planes are z and z^2, respec-

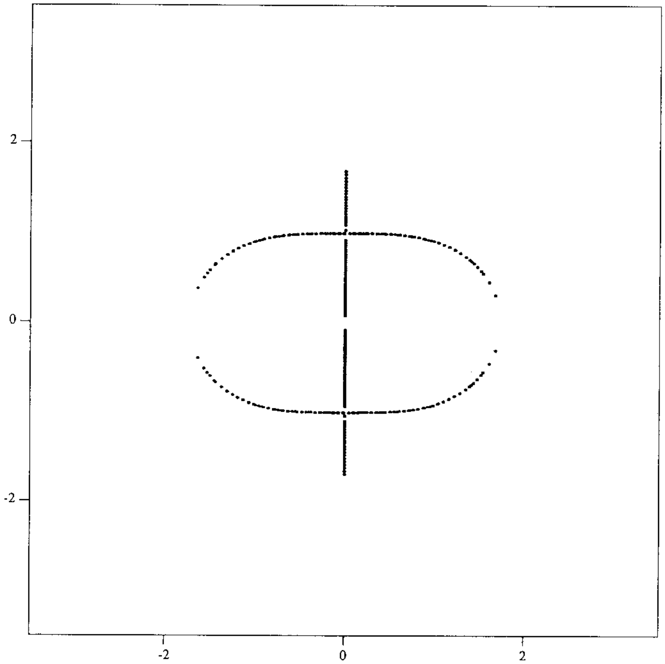

Fig. 1. C_7^{1+} for the $q=2$, 2-site Potts model in the $z=e^K$ plane.

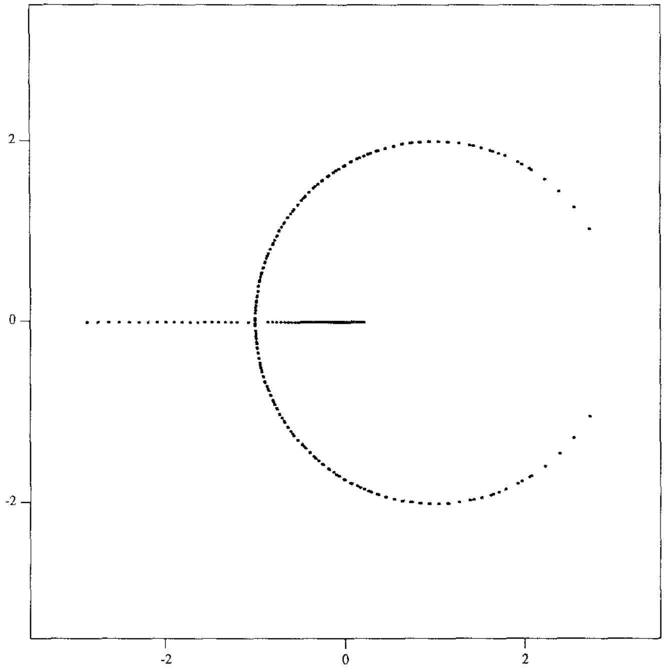

Fig. 2. C_7^{1+} for the $q=2$, 2-site Potts model in the $z^2=e^{2K}$ plane.

tively. Clearly, the latter presents no difficulty; C_7^{1+} on real w is part of the circle

$$z^2 = 1 + 2e^{i\phi} \tag{8}$$

plus a line segment, $|w| \leqslant 1$. So, moving from the z to the z^2 plane uncovers an inversion symmetry. Here C_m^{1+} is always an arc of (8) independent of m, and $z_c^2(m)$ is the *exact* critical point $z_c^2 = 3$, so (7) generates (8) for all m and real w. This invariant circle is of course the consequence of the star-triangle and duality transformations.[10] It is simple to see that if a transformation $z \to z(u)$ leaves (4) invariant under $u \to u^{-1}$ (after the removal of trivial factors from Λ), then the circle $|u| = 1$ will always be generated by (7) on real w. Thus, in the present case at $m=4$, (4) can be put into the form

$$\lambda^4 - 8(2v^2+4v+1)\,\lambda^3 + 64(2v+3)^2\,\lambda^2 - 256(2v^2+4v+1)\,\lambda + 1024 = 0 \tag{9}$$

where λ is a simple multiple of Λ and

$$v = u + u^{-1} \qquad \text{and} \qquad u = \tfrac{1}{2}(z^2 - 1) \tag{10}$$

Conversely, if C_m^{1+} is exactly a circle in some complex plane $g(z)$, then (4) has some form of inversion symmetry. However, what if (7) generates a curve which in some plane $g(z)$ is *very* close to a circle over a sequence of m values? This allows for independent estimates of the center A and radius B and a critical point estimate of $g(z_c) = A + B$. Such behavior suggests that the model may have an inversion symmetry with $u = [g(z) - A]/B$ which becomes exact asymptotically in the limit of $m \to \infty$. In effect, the estimates of the critical point obtained by extending C_m^{1+} onto the real axis are partitioned into two components A and B; thus, $z_c(m) = 2.9820...$ could be more easily recognized as $\frac{5}{4} + \sqrt{3}$ if either A or B could be obtained accurately and independently. This, then, is the present guessing game.

3. POTTS MODELS ON THE TRIANGULAR LATTICE

Our first example is the two-site, q-state Potts model on the triangular lattice, and is chosen to illustrate the phenomena of approximate inversion symmetry. For reference material on Potts models the reader is referred to

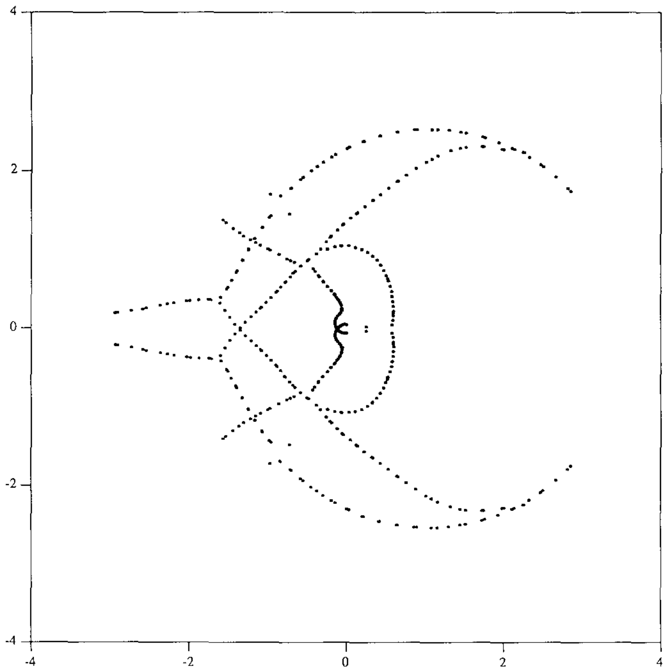

Fig. 3. C_3^{1+} for the $q = 3$, 2-site Potts model in the z^2 plane.

the excellent review by Wu.[11] The critical point of this model is known exactly at $q=2$ and for $q \geqslant 4$ and is given by a root of the equation

$$z^3 - 3z + 2 - q = 0 \qquad (z = e^K) \tag{11}$$

which is also expected to hold at $q=3$. The inversion symmetry of the star-triangle and duality transformations holds only for $q=2$, although a two-variable duality relation is possible for $q \geqslant 2$ *if* the 3-site Potts interaction is added to half of the triangles of the lattice.[11,12] Figures 3–5 show the sequence C_m^{1+} for $q=3$ and $m=3$, 4, and 5, and Figs. 6 and 7 give C_4^{1+} for $q=4$ and 5, respectively. The intersection points $z_c(m)$ obtained by extending the curves through the branch point closest to the positive real axis are listed in Table I.

The full algebraic curves $z(w)$ (w real) obtained from the resolvent (7) are immensely complicated and have many intersection points with the real z axis. Such points correspond to the real branch points of $z(w)$, since they are the meet points of complex conjugate curves. They are also points where the ratio of any pair of eigenvalues obtained from (4) is both real and extremum with respect to real z. Thus, each intersection point can be

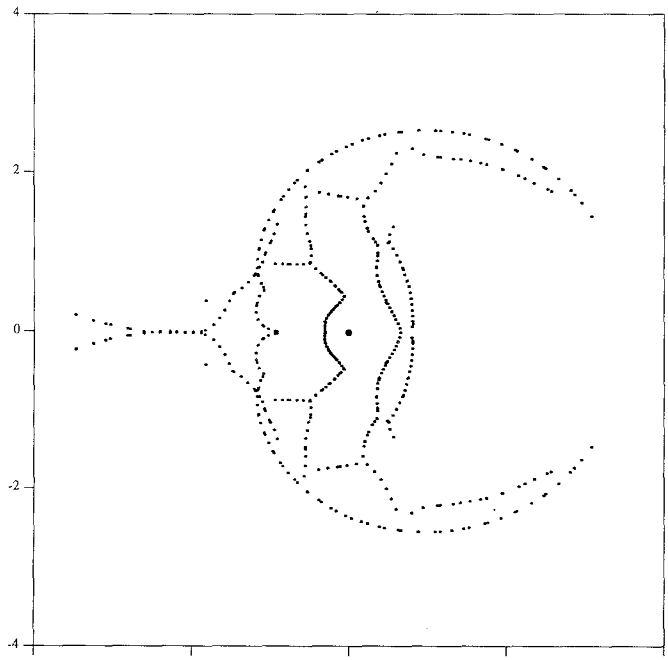

Fig. 4. C_4^{1+} for the $q=3$, 2-site Potts model in the z^2 plane.

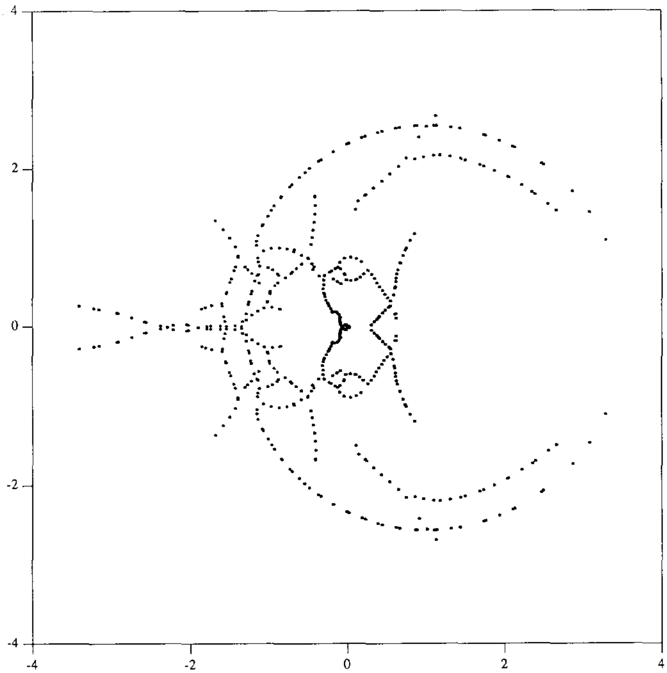

Fig. 5. C_5^{1+} for the $q=3$, 2-site Potts model in the z^2 plane.

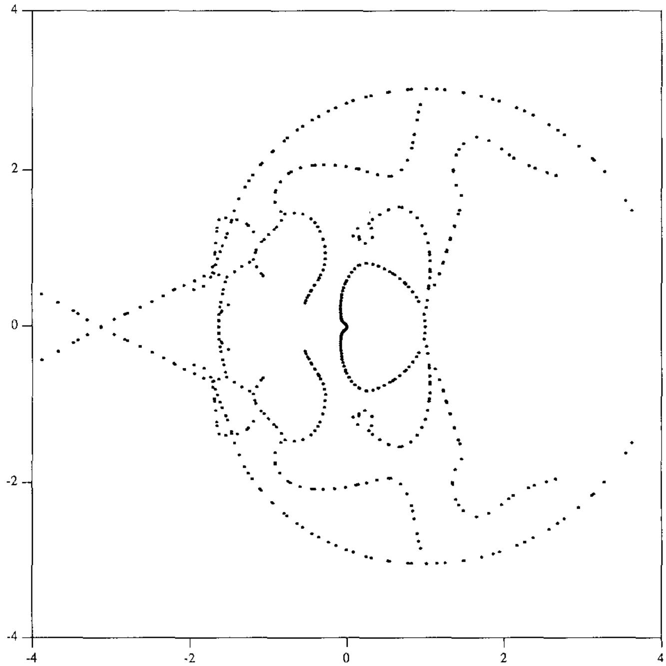

Fig. 6. C_4^{1+} for the $q=4$, 2-site Potts model in the z^2 plane.

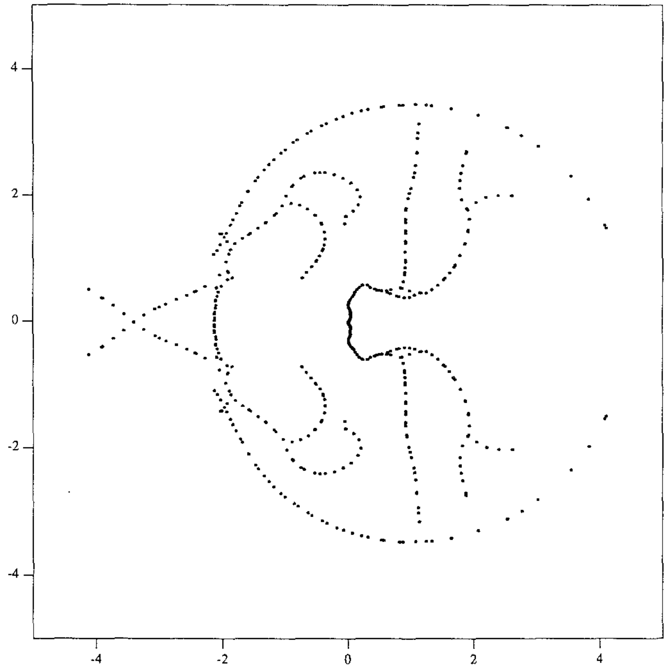

Fig. 7. C_4^{1+} for the $q=5$, 2-state Potts model in the z^2 plane.

associated with a pair (i, j) of function elements of Λ, and we consider these to be ordered in modulus $\Lambda_1^+ > |\Lambda_2| > |\Lambda_3|...$; thus, in Table I the numbers relate to the pair $(1, 2)$. In Table II we list a small selection of such points close to z_c with their associated pair. As can be seen, in a number of cases the intersection points are amazingly close to z_c; for example, the point $z = 1.8793825...$ for the case $q=3$, $m=4$, and $(i, j) = (1, 5)$, where $z_c = 1.8793852$. Any search of the space of irreducible quadratic,

Table I. Approximations to the Critical Point $z_c(m)$ Obtained from C_m^{1+} for the Two-Site Potts Model

m	$q=3$	$q=4$	$q=5$
2	1.8924	2.0593	2.1297
3	1.8836	2.0062	2.1110
4	1.8812	2.0025	2.1067
5	1.8803	2.0013	2.1052
6	1.8799		
∞	1.87938	2	2.10380

Table II. Some Intersection Points Close to z_c Obtained from the Full Algebraic Curve $z(w)$ in (7), for the Two-Site Potts Model

$q=3, m=4$		$q=4, m=5$		$q=5, m=5$	
Pairs (i, j)	Intersections	Pairs (i, j)	Intersections	Pairs (i, j)	Intersections
1, 2	1.8812	1, 2	2.0013	1, 2	2.1052
1, 3	1.8716	1, 3	2.0001	1, 3	2.1057
1, 4	1.8856	1, 4	2.0036	1, 5	2.1034
1, 5	1.8793825...	1, 5	1.9996	1, 7	2.1040
4, 5	1.8749	1, 9	1.9999	1, 10	2.10381

cubic, and quartic equations with "small" integer coefficients would *immediately* reveal (11) at $q=3$ using this intersection point; similarly the point from (1, 10) at $q=5$, $m=5$. In the hard-hexagon model many such (i, j) pairs exist with intersection points occurring at the exact roots of (1).[4]

The outer curves in C_m^{1+} shown in Figs. 3–7 clearly appear to contain the arcs of a circle; if corresponding members of a sequence are overlaid

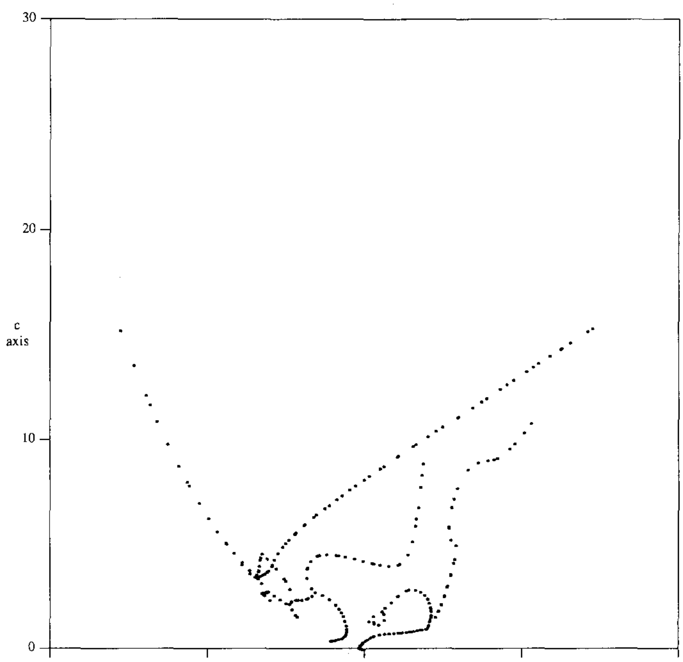

Fig. 8. A b–c plot for C_4^{1+} in Fig. 4.

they are indistinguishable in the right half-plane. The various branches of C_m^{1+} derive from a quadratic factor

$$z^2 - b(w)\, z + c(w) = 0 \tag{12}$$

in the resolvent (7). Thus, if

$$z = A + Be^{\pm i\theta} \tag{13}$$

are the roots of such a factor, then

$$c = Ab + (B^2 - A^2) \tag{14}$$

Taking $c = |z|^2$ and $b = 2$ (real part of z) from points in C_m^{1+}, we obtain a b–c plot which provides a measure of the closeness of fit to arcs with quadratic curvature in C_m^{1+}, and correspondingly estimates of the center and radius. Figures 8–10 show the b–c plots for $m=4$ and $q=3, 4$, and 5, respectively. The higher m values of 5 and 6 are indistinguishable from these plots, which clearly have an impressively linear section relating to the outer arc of C_4^{1+}. It is impossible to avoid the speculation that the two-site

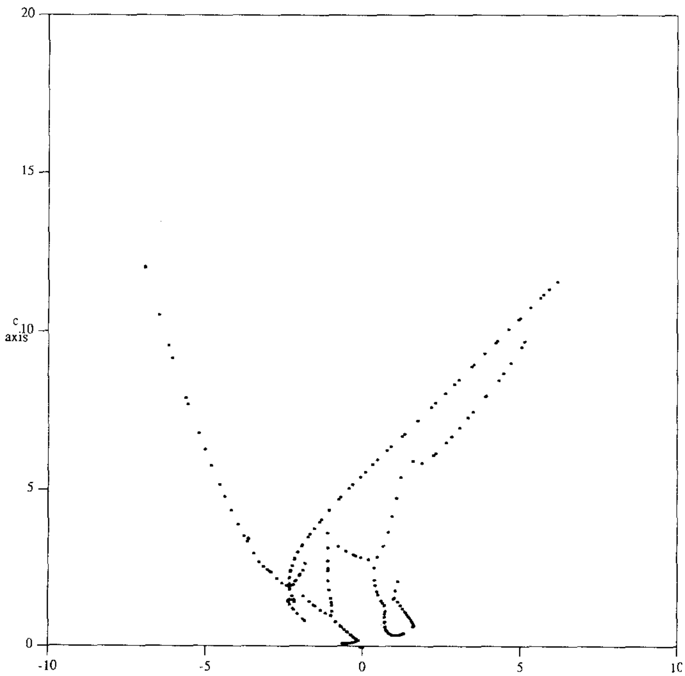

Fig. 9. A b–c plot for C_4^{1+} in Fig. 6.

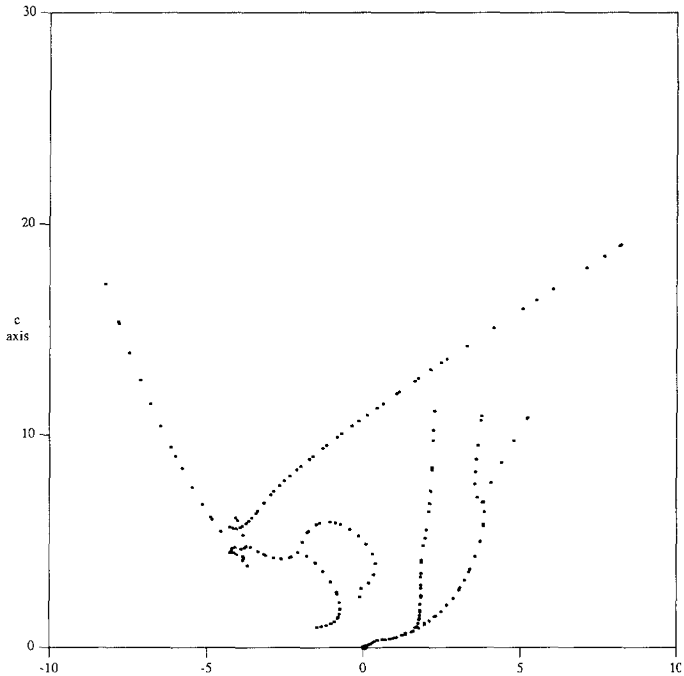

Fig. 10. A b–c plot for C_4^{1+} in Fig. 7.

Potts model on the triangular lattice has an asymptotic inversion symmetry in the variable u given by

$$z^2 = 1 + [z_c^2(q) - 1]\, u \tag{15}$$

where $|u| = 1$ is C_m^{1+} in the limit of $m \to \infty$.

Our second example is the three-site Potts model on the triangular lattice, where the three-site Potts term $L\delta(\sigma, \sigma', \sigma'')$ $(\sigma = 1, 2,..., q)$ exists on all the triangles of the lattice.[11] Here the critical point is *not* known. The model was the occasion of a conjecture by Wu[13] that the critical point was simply given by

$$z_c^2 = 1 + q \qquad (z = e^L) \tag{16}$$

but this was shown to be incorrect by Enting and Wu[14] in a study of the $q = 3$ case. The same model in which interactions exist in only half of the triangles does have an inversion symmetry through a self-duality transformation and the curves C_m^{1+} are arcs on the invariant circle

$$z = 1 + qe^{i\theta} \qquad (z = e^L) \tag{17}$$

Thus, if (16) had been true, this inversion symmetry would have simply shifted from the z plane to the z^2 plane. Our calculations at finite values of m show that in fact the model appears to be *very* close indeed to an inversion symmetry in the z^2 plane in the form

$$z^2 = A(q) + qu \tag{18}$$

and C_m^{1+} extraordinarily close to a circle of radius q, but with centers $A(q)$ which drift away from $z = 1$ for $q > 2$. This shift is quite small for $q = 3$, which explains why the series expansion estimate of z_c obtained by Enting and Wu[14] ($e^{-L} = 0.5038 \pm 0.0005$) is close to 2, and the conjecture (16), which in a sense is correct with regard to the appearance of q.

In Figures 11–13 we show C_5^{1+} for $q = 3$, 4, and 5; the corresponding b–c plots are impressively linear. Taking the curvature from the neighborhood of the branch point, the radii are estimated, respectively, at 2.97, 3.99, and 5.04. We adopt the conjecture that C_m^{1+} asymptotically converges to a circle of radius q in the z^2 plane. The approximations to z_c obtained through $z_c(m)$ are shown in Table III. Some detective work on $A(q)$ in (18) remains. The values of $z_5(m)$ in Table III are almost certainly

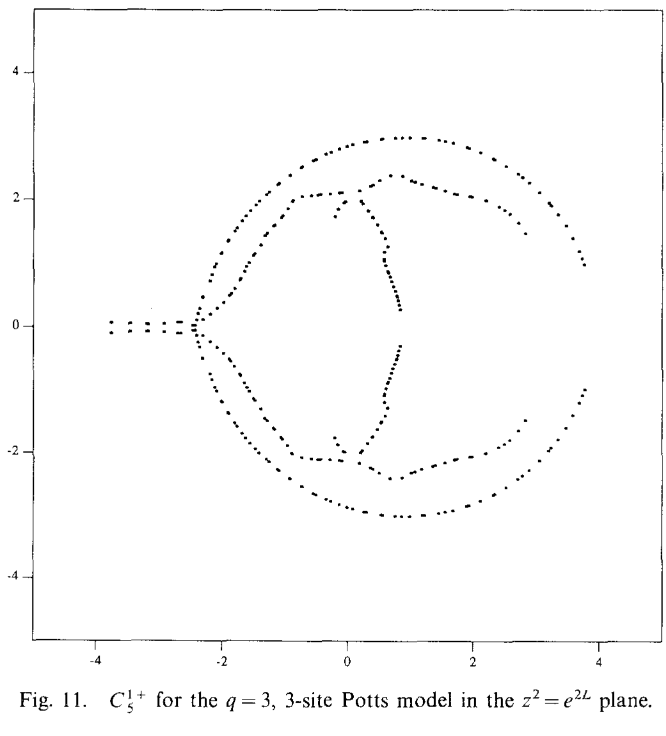

Fig. 11. C_5^{1+} for the $q = 3$, 3-site Potts model in the $z^2 = e^{2L}$ plane.

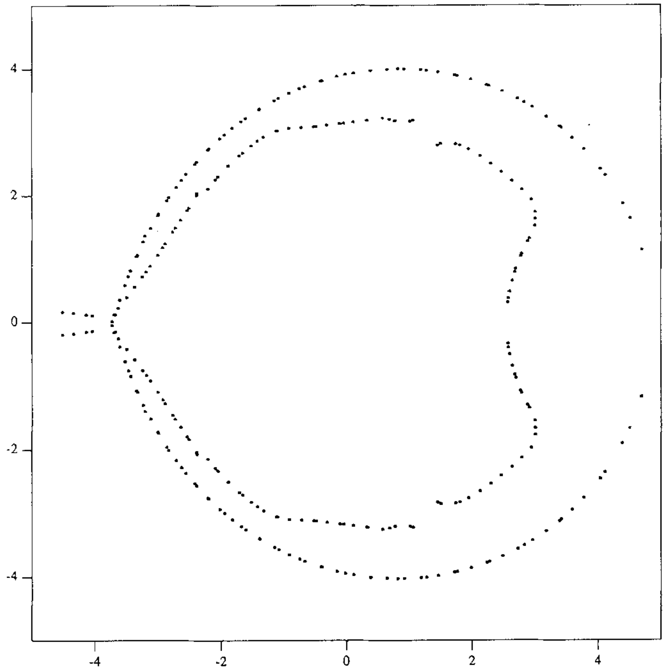

Fig. 12. C_5^{1+} for the $q=4$, 3-site Potts model in the $z^2=e^{2L}$ plane.

correct to order 10^{-3}, and in the case of $q=4$ we have two intersections at 2.20568..., which is probably very close to the exact value. Thus, $z_c(5)-q$ probably estimates $A(q)$ in (18) to 10^{-3}, and on this basis it is fairly easy to tease out the conjecture

$$z_c^2=\left(\frac{\sqrt{3}}{2}\right)^{(q-2)/2}+q \tag{19}$$

The conjectured values are listed in Table III. In addition, the correct value $z_c^2=3$ is recovered at $q=2$ and a further test is available at $q=1$, where the model has a percolation limit on the honeycomb lattice.[15] Monte Carlo RG finite-size scaling calculations were carried out by Vicsek and Kertész,[15] who reported a value of the critical probability corresponding to z_c of

$$z_c^{-1}=0.6973\pm 0.0008 \tag{20}$$

and observed it to be in disagreement with (16). At $q=1$, (19) yields the value

$$z_c^{-1}=0.69428... \tag{21}$$

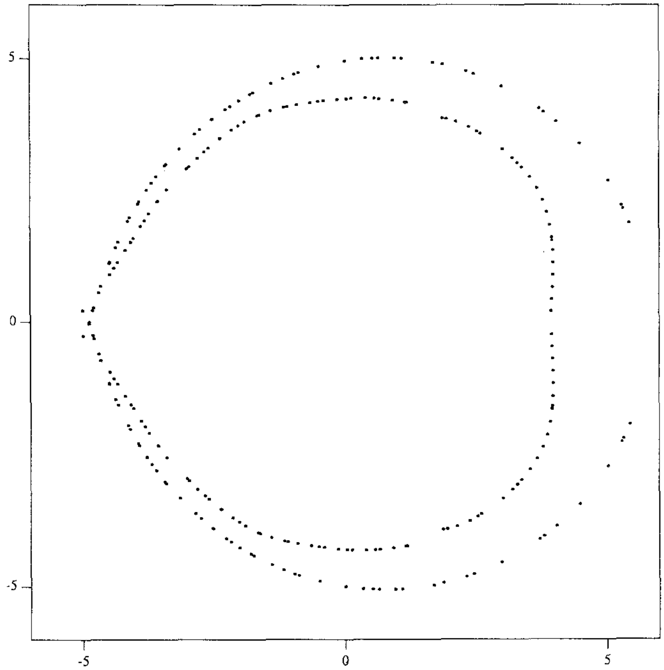

Fig. 13. C_5^{1+} for the $q=5$, 3-site Potts model in the $z^2=e^{2L}$ plane.

and, in view of Table III, we assume that the "confidence limits" in (20) are a little overconfident.

As a final comment on algebraic critical points, one of us (D.W.W.) adds an observation on the directed percolation problem on the square net lattice and on the hard-square gas. In recent series expansion work Baxter and Guttmann[16] report an estimate of the critical probability

$$p_c = 0.644701 \pm 0.000001. \tag{22}$$

Table III. Approximations to the Critical Point z_c Obtained from the Intersection Points $z_c(m)$

m	$q=3$	$q=4$	$q=5$
3	1.9818	2.205683	2.4106
4	1.98219	2.2056	2.40997
5	1.98242	2.205685	2.40984
Eq. (19)	1.982575...	2.205906...	2.409549...

While considering work on this model of a similar nature to that reported in this paper, it was observed that the equation

$$\sqrt{q_c}\,(q_c+3)=2 \qquad (p_c+q_c=1) \tag{23}$$

has a root at

$$\sqrt{q_c}=(1+\sqrt{2})^{1/3}+(1-\sqrt{2})^{1/3} \tag{24}$$

corresponding to a value of

$$p_c=0.6446986... \tag{25}$$

On such occasions one has to ask what meaning does one attach to the term "confidence limit"?—one would so love to know!

The hard-square-gas problem[3,17] has failed to yield any exact critical parameters. The grand canonical partition function clearly has two real singular points in the activity plane, a physical singularity z_c and a non-physical singularity $z_{\rm NP}$. Attempts to uncover a critical point equation similar to (1) using Gaunt's trick[3] or the technique described by Wood and Turnbull[4] have failed; consequently, the following observation may be of interest. The two singular points have been estimated to have the values[17,18]

$$z_c=3.7962\pm 0.0001 \tag{26}$$

and

$$z_{\rm NP}=-0.1193388809\pm 0.000{,}000{,}001. \tag{27}$$

Taking (27) to 4 d.p., one observes that

$$\sqrt{2}\,(z_c+z_{\rm NP})=5.1999 \tag{28}$$

suggesting the symmetric sum $5+\frac{1}{5}$ (Kleinian theorists please note). The remaining part of the algorithm is left as an exercise for the reader.

REFERENCES

1. W. Wordsworth, "Intimations of Immortality from Recollections of Early Childhood," in *Poems in Two Volumes* (1807).
2. C. Domb, Critical phenomena, in *Proceedings Conference Washington DC 1965*, M. S. Green and J. V. Sengers, eds. (1966), p. 29.
3. R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, New York, 1982), p. 405.
4. D. W. Wood and R. W. Turnbull, *J. Phys. A* **21**:L989 (1988).

5. D. W. Wood, *J. Phys. A* **20**:3471 (1987).
6. D. W. Wood, R. W. Turnbull, and J. K. Ball, *J. Phys. A* **20**:3495 (1987).
7. D. W. Wood, in *Proceedings 10th Annual Open University Conference on Statistical Mechanics*, A. I. Solomon, ed. (World Scientific, Singapore, 1988).
8. D. W. Wood, R. W. Turnbull, and J. K. Ball, *J. Phys. A* **22**:L109 (1989).
9. D. W. Wood, in *Proceedings XVII International Conference on Differential Geometric Methods in Theoretical Physics* (World Scientific, Singapore, 1989).
10. C. Domb, *Adv. Phys.* **9**:149 (1960).
11. F. Y. Wu, *Rev. Mod. Phys.* **54**:235 (1982).
12. D. Kim and R. I. Joseph, *J. Phys. C* **7**:L167 (1974).
13. F. Y. Wu, *J. Phys. C* **12**:L645 (1979).
14. I. G. Enting and F. Y. Wu, *J. Stat. Phys.* **28**:351 (1982).
15. T. Vicsek and J. Kertész, *Phys. Lett.* **81A**:51 (1981).
16. R. J. Baxter and A. J. Guttman, *J. Phys. A* **21**:3193 (1988).
17. R. J. Baxter, I. G. Enting, and S. K. Tsang, *J. Stat. Phys.* **22**:465 (1980).
18. A. J. Guttmann, *J. Phys. A* **20**:511 (1987).