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1989 J. Phys. A: Math. Gen. 22 L105

(http://iopscience.iop.org/0305-4470/22/3/008)

J. Phys. A: Math. Gen. 22 (1989) L105–L109. Printed in the UK

LETTER TO THE EDITOR

# An observation on the partition function zeros of the hard hexagon model

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Received 21 October 1988

**Abstract.** It is conjectured that part of the limiting locus of partition function zeros for the hard hexagon model is an algebraic curve generated by a simple and rational algebraic equation. This equation arises from the same mathematical mechanism as that which determines algebraic-invariant properties of self-dual systems. A remarkable approximation to the critical point of the three-state Potts model (triangular lattice) is mentioned in passing.

The observation reported here originates from a combination of recent work in the theory of critical phenomena by the present authors (Wood 1987, 1988, Wood *et al* 1987, Wood and Turnbull 1988) and the recent work of Joyce (1988) on the thermodynamic functions of the hard hexagon model, which suggests that the limiting locus of partition function zeros for the hard hexagon model is determined by a simple algebraic equation. The work of the present authors seeks to understand the emergence of critical-point phenomena in the thermodynamic limit in terms of the sequence of algebraic functions $\Lambda_1(m, z)$ which determine the partition functions of a sequence of semi-infinite $m \times \infty$ lattice sections. The $m \to \infty$ limit of this function sequence defines the partition function per site $Z(z)$ of the model

$$Z(z) = \lim_{m\to\infty} (\Lambda_1^+(m, z))^{1/m} \tag{1}$$

where $\Lambda_1^+(m, z)$ is the function element of $\Lambda_1(m, z)$ which is maximum in modulus on the real positive $z$ axis, and $z$ is some suitable temperature variable.

For the hard hexagon model the partition function is the grand canonical partition function $\Xi$ and $z$ is the activity variable. Joyce's work has shown that for this model the limit $\Xi(z)$ given by (1) is also an algebraic function in the sense that it is a function element of an algebraic equation. For $m$ finite it is possible to find the limiting locus of zeros of a block partition function (see equation (4)) in terms of the function elements of $\Lambda_1(m, z)$ (Wood 1987). This locus is an algebraic curve denoted by $C_m^{1+}$, in the limit of $m \to \infty$ it is envisaged that this sequence of algebraic curves will converge onto a limiting curve $C_\infty$; this curve and the distribution of zeros on it define the partition functions per site in (1). The question arises as to whether $C_\infty$ can be obtained from the function elements of Joyce's algebraic equation for $\Xi(z)$. We believe that the numerical evidence given here suggests that $C_\infty$ can be found in this way; if this is so then the mathematical mechanism which locates $C_\infty$ is especially interesting since it is precisely the mechanism which appears in models with self-dual symmetry, namely simple complex conjugation of roots of algebraic equations.

Let $T_m(z)$ be the transfer matrix relating to an $m \times \infty$ lattice strip. The characteristic equation of $T_m(z)$ can be factored into irreducible polynomial factors $P_k(z, \Lambda_k)$ in the form

$$|T_m(z) - \Lambda I| = \prod_k P_k(z, \Lambda_k). \tag{2}$$

The algebraic function $\Lambda_1(m, z)$ is determined by the polynomial equation

$$P_1(z, \Lambda_1) = \sum_{r=0}^{s} \phi_r(z)\Lambda_1^{s-r} = 0 \tag{3}$$

which is the characteristic equation of a block $\tau_1(z, m)$ obtained in a block diagonalisation of $T_m(z)$, and where $\phi_r(z)$ are polynomials. We use the block $\tau_1(z, m)$ to define the block partition function $Z_{mn}^{(1)}(z)$ for an $m \times n$ lattice as

$$Z_{mn}^{(1)}(z) = \mathrm{Tr}(\tau_1(z, m))^n. \tag{4}$$

The block partition function per site of the $m \times \infty$ section is equal to the partition function per site which is $(\Lambda_1^+(m, z))^{1/m}$. In the limit of $n \to \infty$ ($Z_{mn}^{(1)}$ is a polynomial in $z$ with positive coefficients) the zeros of the block partition function lie on an algebraic curve $C_m^{1+}$ determined by the function elements $z(h)$ of the polynomial resolvent equation (see Wood 1987)

$$R(h, z) = \sum_{\alpha\beta} A_{\alpha\beta} z^\alpha h^\beta = 0 \tag{5}$$

where the $A_{\alpha\beta}$ are integers and $|h| = 1$. For a fixed $h$ the function elements $z(h)$ of the algebraic function defined by (5) locate points in the $z$ plane where the function elements of $\Lambda_1$ contain pairs which are in ratio $h$. The algebraic curve $C_m^{1+}$ is a cut in the $z$ plane joining the branch points of $\Lambda_1$ where the function elements are simultaneously equal and maximum in modulus. For the hard hexagon model and $m = 12$ this curve is shown in figure 1 where • denotes a branch point.

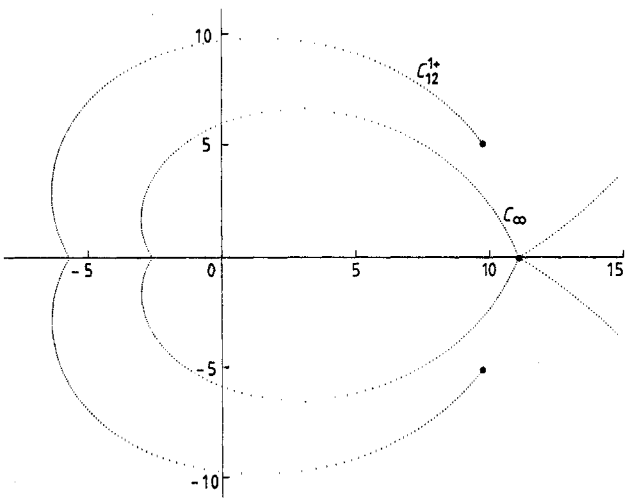


**Figure 1.** The algebraic curve $C_{12}^{1+}$ and the section of the algebraic curve generated by the algebraic equation (18) which is conjectured to be part of $C_\infty$.

Consider now a typical self-dual system such as the $q$-state Potts model (see Wu 1982) on the square lattice where on an $m\times n$ toroidal lattice the partition function $Z_{mn}$ satisfies the duality relation

$$Z_{mn}(q,z)=\left(\frac{z-1}{\sqrt{q}}\right)^{2mn} Z_{mn}(q,z^*) \tag{6}$$

where $z=e^K$ and

$$(z-1)(z^*-1)=q. \tag{7}$$

In the limit of $n\to\infty$, and defining the duality variable $u$ by $z=1+\sqrt{q}u$ $(u^*=u^{-1})$ equation (6) becomes

$$(u^{-1})^m\Lambda_1^+(q,u,m)=u^m\Lambda_1^+(q,u^{-1},m). \tag{8}$$

Hence we see that if we write the characteristic equation (3) in terms of the variable $y=u^{-m}\Lambda_1$ the whole equation must be invariant under the transformation $u\to u^{-1}$ and it will always be possible to write (3) in the reduced form

$$\sum_{r=0}^{s}\Phi_r(q,w)y^{s-r}=0 \tag{9}$$

where $w=u+u^{-1}$.

We can now guess part of the geometry of $C_m^{1+}$ by inspection since for real $w$ the function elements of $y$ are either real or in complex conjugate pairs, hence the roots of (5) on the domain of $|h|=1$ and $h$ real contain the whole circle $z=1+\sqrt{q}\,e^{i\theta}$ (where $w=2\cos\theta$) for all $m$; $C_m^{1+}$ will be an arc of this circle *if* a branch point of $\Lambda_1^+(m,z)$ lies on the circle. Numerical work suggests that this is always the case and indeed that the ferromagnetic critical point at $z_c=1+\sqrt{q}$ is the limit point of a sequence of such branch points moving along this circle and converging onto $z_c$ in the limit of $m\to\infty$. The exact critical point is in fact a value of $z$ corresponding to an algebraic singular point of $z(h)$ defined by (5) (see Wood *et al* 1987). We have frequently observed that for most models such algebraic singular points often lie very close to the true critical point (in the case of the hard hexagon model the true critical point appears to be invariantly a singular point of $z(h)$ (Wood and Turnbull 1988)). We mention in passing a recent example of this phenomenon found for the three-state Potts model on the triangular lattice where a singular point in $z(h)$ at $m=4$ corresponds to a value of $z=1.879\,382\,463\ldots$. The true critical point is believed to be the root of the equation $z^3-3z-1=0$ at $z=1.879\,385\,24\ldots$(!). In summary the mechanism which defines $C_m^{1+}$ and an invariant part of $C_\infty$ is simply the complex conjugation of roots in a reduced characteristic equation along a curve in the $z$ plane determined by a rational algebraic equation, which for the Potts model is the equation

$$u^2-wu+1=0 \tag{10}$$

for real $w$.

Now we can consider Joyce's result for the hard hexagon model, namely that $\Xi(z)$, for real $z$ in the high-density regime $z\geqslant z_c$, is a function element of the algebraic equation

$$(z')^2\Omega_1^{10}(z')y^4-\Omega_3(z')(1458z'\Omega_1^5(z')+\Omega_3^2(z'))y^3 \\ -3^{10}(2430z'\Omega_1^5(z')+\Omega_3^2(z'))y^2-3^{19}\Omega_3(z')y-3^{27}=0 \tag{11}$$

where $z' = z^{-1}$ and

$$y = \Xi^6 \tag{12}$$

and $\Omega_1$ and $\Omega_3$ are the polynomials

$$\Omega_1(z') = 1 - 11z' - (z')^2 \tag{13}$$

$$\Omega_3(z') = 1 - 522z' - 10005(z')^2 - 10005(z')^4 + 522(z')^5 + (z')^6. \tag{14}$$

Equation (11) of Joyce (1988) can be parametrised by the rational function

$$w = z'\Omega_1^5(z')/\Omega_3^2(z') \tag{15}$$

since on writing

$$y = -3^9\lambda/\Omega_3 \tag{16}$$

we obtain the reduced algebraic equation

$$3^9w^2\lambda^4 + 1458w\lambda^3 - 7290w\lambda^2 + (\lambda - 1)^3 = 0. \tag{17}$$

Equation (17) highlights the branch points of cycle number 3 occurring at the zeros of $w$, which are at the two singular points of $\Xi$, $z = \frac{1}{2}(11 \pm 5\sqrt{5})$, and at $z = 0$ and $\infty$.

One naturally speculates on how (or if) the algebraic equation (11) emerges from the sequence of algebraic equations (3) in the limit of $m \to \infty$ where on writing $\Lambda_1(m, z) = \{\Xi(m, z)\}^m$ one branch of (3) is the partition function per site of the $m \times \infty$ strip. We know that for sufficiently large $m$ a branch of (3) can be made arbitrarily close to the partition function per site $\Xi$ obtained from (11). Are other branches of (3) also convergent upon any of the other branches of (11)? At sufficiently large $m$ the endpoints of $C_m^{1+}$ (and branch points of $\Lambda_1^+$) can be made arbitrarily close to the two real singular points $z = \frac{1}{2}(11 \pm 5\sqrt{5})$ and it seems reasonable to suppose that the function elements of (3) participating in these branch points are also close approximations to the branches of (11) participating in the branch point at $z_c$. Thus we expect that $C_m^{1+}$ would contain an algebraic curve convergent upon some section of the algebraic curves generated by the resolvent function (5) *defined on the algebraic equation* (11). The reduction of (11) to (17) re-establishes the situation occurring with self-dual systems in that we can guess by inspection some of the algebraic curves from this resolvent. The analogue of (10) is the rational algebraic equation

$$z'\Omega_1^5(z') = w\Omega_3^2(z') \tag{18}$$

(where $w$ is real) tracing out an algebraic curve through the function elements $z(w)$. Those sections of these curves along which complex conjugate roots of (17) are simultaneously maximum in modulus, we would conjecture to be part of $C_\infty$; we have shown this curve in figure 1 labelled as $C_\infty$. This curve is neatly nested inside $C_{12}^{1+}$ and clearly appears to be a scaled version of it. Extending $C_{12}^{1+}$ by adding the domain $h$ real to (5) produces a smooth continuation through the branch point • to an orthogonal intersection with the real axis at $z = 11.1331\ldots$ ($z_c = 11.09017\ldots$).

The curve $C_\infty$ in figure 1 approaches the real critical point along two pairs of complex conjugate curves making angles of $\frac{2}{5}\pi$, and $\frac{4}{5}\pi$ with the negative real axis direction. The two prongs which are terminated in figure 1 describe another closed loop meeting the negative axis at a large distance from the origin. If the curve $C_\infty$ approached $z_c$ along only *one pair* of complex conjugate curves then we would expect an orthogonal crossing of the real axis at $z_c$. This is based on the scaling conjecture of Itzykson *et al* (1983) that the angle of contact $\phi$ with the negative $z$ axis is given by

$$\tan[(2-\alpha)\phi] = (\cos \pi\alpha - A_-/A_+)/\sin \pi\alpha \tag{19}$$

where $\alpha$ is the specific heat exponent and $A_+$, $A_-$ are the coefficients in the leading singular terms in the free energy. For the hard hexagon model $\alpha = \frac{1}{3}$ and $A_+ = A_-$ (Baxter 1982).

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