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LETTER TO THE EDITOR

On the icosahedral equation and the locus of zeros for the grand partition function of the hard-hexagon model

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Abstract. The Kleinian theory of the icosahedral equation is used to investigate a recent conjecture on the locus of zeros for the grand partition function of the hard-hexagon lattice gas model.

Baxter (1980, 1981) has shown that in the thermodynamic limit the grand partition function per site Ξ of the hard-hexagon lattice gas model has a parametric representation in the ordered regime given by

$$\Xi = x^{-1/3}\frac{G^3(x)}{H^2(x)}\prod_{n=1}^{\infty}\frac{(1-x^{3n-2})(1-x^{3n-1})(1-x^{5n})^2}{(1-x^{3n})^2} \tag{1}$$

$$z^{-1} = x[H(x)/G(x)]^5 \tag{2}$$

where z is the activity of the gas, and

$$G(x) = \prod_{n=1}^{\infty}[(1-x^{5n-4})(1-x^{5n-1})]^{-1} \tag{3}$$

$$H(x) = \prod_{n=1}^{\infty}[(1-x^{5n-3})(1-x^{5n-2})]^{-1} \tag{4}$$

and $0<x<1$. When $x\to 1-$ the model displays an order-disorder transition with a critical activity value

$$z_c = [\tfrac{1}{2}(1+\sqrt{5})]^5. \tag{5}$$

Similar results were also obtained by Baxter for the disordered regime $0\leqslant z<z_c$.

Recently, Joyce (1988) has used the theory of modular functions to eliminate the non-physical parameter x from equations (1) and (2). It was found that the grand partition function is an *algebraic* function $\Xi(z')$ of the reciprocal activity $z'=z^{-1}$ which satisfies the polynomial equation

$$(z')^2\Omega_1^{10}(z')y^4 - \Omega_3(z')[1458z'\Omega_1^5(z')+\Omega_3^2(z')]y^3 - 3^{10}[2430z'\Omega_1^5(z')+\Omega_3^2(z')]y^2 - 3^{19}\Omega_3(z')y - 3^{27} = 0 \tag{6}$$

where

$$y = \Xi^6 \tag{7}$$

$$\Omega_1(z') = 1-11z'-(z')^2 \tag{8}$$

$$\Omega_3(z') = 1-522z'-10\,005(z')^2-10\,005(z')^4+522(z')^5+(z')^6. \tag{9}$$

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Wood *et al* (1989) have investigated the resolvent properties of the polynomial equation (6) and have *conjectured* that part of the limiting locus of grand partition function zeros in the z plane for the hard-hexagon model can be generated by considering the solutions $z = z(w)$ of the rational algebraic equation

$$w = z'\Omega_1^5(z')/\Omega_3^2(z') \tag{10}$$

where w is a *real* parameter.

The main purpose in this letter is to investigate the mathematical properties of the solutions $z = z(w)$ of equation (10). In particular, it will be shown that the algebraic curves generated by the solutions $z = z(w)$ have simple *rational* parametric representations. We begin the analysis by considering the following basic modular functions (Klein and Fricke 1890, p 154, 1892, p 383):

$$J(\tau) = (1728x)^{-1}\left[1 + 240\sum_{n=1}^{\infty} n^3x^n(1-x^n)^{-1}\right]^3 \prod_{n=1}^{\infty}(1-x^n)^{-24} \tag{11}$$

$$\zeta(\tau) = x^{1/5}H(x)/G(x) \tag{12}$$

where

$$x = \exp(2\pi \mathrm{i}\tau) \tag{13}$$

and the variable τ lies in the upper half-plane $\mathrm{Im}(\tau) > 0$. The function $J(\tau)$ is the fundamental hauptmodul for the full modular group Γ, and $\zeta(\tau)$ is the hauptmodul for the principal congruence subgroup $\Gamma(5)$. Because the function $J(\tau)$ is a modular invariant for all the transformations belonging to $\Gamma(5)$ it is possible to write $J(\tau)$ as a rational function of $\zeta(\tau)$. In fact Klein and Fricke (1890, p 105) have proved that this rational relation can be expressed in the two *equivalent* forms:

$$1728J = \Omega_2^3(\zeta^5)/\zeta^5\Omega_1^5(\zeta^5) \tag{14}$$

$$1728(J-1) = \Omega_3^2(\zeta^5)/\zeta^5\Omega_1^5(\zeta^5) \tag{15}$$

where

$$\Omega_2(\zeta^5) = 1 + 228\zeta^5 + 494\zeta^{10} - 228\zeta^{15} + \zeta^{20} \tag{16}$$

and the polynomials Ω_1 and Ω_3 are defined in equations (8) and (9) respectively.

Equation (14) defines an algebraic inverse function $\zeta(J)$ which consists of 60 function elements, and has a Galois group which is isomorphic with the icosahedral rotation group (Klein 1913). It is also known that the zeros of the polynomials $\Omega_j(\zeta^5)$ $(j = 1, 2, 3)$ are closely connected with the geometrical properties of the icosahedron. Because of these remarkable properties equations (14) and (15) are, not surprisingly, referred to as the *icosahedral* equations. If we now make the identifications

$$z' = z^{-1} \equiv \zeta^5 \tag{17}$$

$$w^{-1} \equiv 1728(J-1) \tag{18}$$

we see that the basic equation (10) becomes the icosahedral equation (15) with J *real.*

Unfortunately, the icosahedral equation (15) is *not* solvable in terms of radicals because the Galois group for the equation is *simple.* However, it is possible to express the inverse function $\zeta(J)$ in terms of hypergeometric series by using the work of Schwarz (1873). In this manner we find that *one* solution of the equation is

$$\zeta_0(J) = (12)^{-3/5}\,\mathrm{sgn}(J)|J|^{-1/5}F_1/F_2 \tag{19}$$

where

$$F_1 \equiv {}_2F_1(\tfrac{11}{60}, \tfrac{31}{60}; \tfrac{6}{5}; 1/J) \tag{20}$$

$$F_2 \equiv {}_2F_1(-\tfrac{1}{60}, \tfrac{19}{60}; \tfrac{4}{5}; 1/J) \tag{21}$$

and $1 \leqslant |J| < \infty$, with J real. The application of the transformation formula (Erdélyi *et al* 1953, p 105)

$${}_2F_1(a, b; c; z) = (1-z)^{-a}{}_2F_1[a, c-b; c; z/(z-1)] \tag{22}$$

to equation (19) yields the alternative expression

$$\zeta_0(J) = (12)^{-3/5}\,\mathrm{sgn}(J-1)|J-1|^{-1/5}F_3/F_4 \tag{23}$$

where

$$F_3 \equiv {}_2F_1(\tfrac{11}{60}, \tfrac{41}{60}; \tfrac{6}{5}; 1/(1-J)) \tag{24}$$

$$F_4 \equiv {}_2F_1(-\tfrac{1}{60}, \tfrac{29}{60}; \tfrac{4}{5}; 1/(1-J)) \tag{25}$$

and $-\infty < J \leqslant 0$ or $J > 2$. It is clear that equation (23) is particularly useful for the case $J \leqslant 0$.

We can determine the behaviour of $\zeta_0(J)$ in the neighbourhood of the branch point $J = 1$ by applying standard analytic continuation formulae (Erdélyi *et al* 1953, pp 105, 108) to equation (19). The final result is

$$\zeta_0(J) = A_1[F_5 - A_2(J-1)^{1/2}F_6]/[F_5 + A_3(J-1)^{1/2}F_6] \tag{26}$$

where

$$F_5 \equiv {}_2F_1(-\tfrac{1}{60}, \tfrac{11}{60}; \tfrac{1}{2}; 1-J) \tag{27}$$

$$F_6 \equiv {}_2F_1(\tfrac{29}{60}, \tfrac{41}{60}; \tfrac{3}{2}; 1-J) \tag{28}$$

$$A_1 = 2^{-1}[-(1+\surd 5) + \surd 2(5+\surd 5)^{1/2}] \tag{29}$$

$$A_2 = 2^{-2}3^{-1/2}5^{-3/4}[(1+\surd 5) + \surd 2(5+\surd 5)^{1/2}] \tag{30}$$

$$A_3 = 2^{-2}3^{-1/2}5^{-3/4}[-(1+\surd 5) + \surd 2(5+\surd 5)^{1/2}] \tag{31}$$

and $1 \leqslant J \leqslant 2$. A similar procedure can be used to establish the behaviour of $\zeta_0(J)$ in the neighbourhood of the branch point $J = 0$. It is found that

$$\zeta_0(J) = -A_4[F_7 + A_5\,\mathrm{sgn}(J)|J|^{1/3}F_8]/[F_7 - A_6\,\mathrm{sgn}(J)|J|^{1/3}F_8] \tag{32}$$

where

$$F_7 \equiv {}_2F_1(-\tfrac{1}{60}, \tfrac{11}{60}; \tfrac{2}{3}; J) \tag{33}$$

$$F_8 \equiv {}_2F_1(\tfrac{19}{60}, \tfrac{31}{60}; \tfrac{4}{3}; J) \tag{34}$$

$$A_4 = 2^{-2}[-(3+\surd 5) + \surd 6(5+\surd 5)^{1/2}] \tag{35}$$

$$A_5 = 2^{-3}5^{-5/6}[(3+\surd 5) + \surd 6(5+\surd 5)^{1/2}] \tag{36}$$

$$A_6 = 2^{-3}5^{-5/6}[-(3+\surd 5) + \surd 6(5+\surd 5)^{1/2}] \tag{37}$$

and $-1 \leqslant J < 1$. Finally, we note that the behaviour of the solution (32) in the neighbourhood of $J = 1$ is given by the formula

$$\zeta_0(J) = -A_7[F_5 - A_8(1-J)^{1/2}F_6]/[F_5 + A_9(1-J)^{1/2}F_6] \tag{38}$$

where

$$A_7 = 2^{-1}[(1-\sqrt{5})+\sqrt{2}(5-\sqrt{5})^{1/2}] \tag{39}$$

$$A_8 = 2^{-2}3^{-1/2}5^{-3/4}[-(1-\sqrt{5})+\sqrt{2}(5-\sqrt{5})^{1/2}] \tag{40}$$

$$A_9 = 2^{-2}3^{-1/2}5^{-3/4}[(1-\sqrt{5})+\sqrt{2}(5-\sqrt{5})^{1/2}] \tag{41}$$

and $0 \leq J < 1$. We have now constructed *one* real root $\zeta_0(J)$ of the icosahedral equation for each real value of J. It should be pointed out, however, that the various formulae given for $\zeta_0(J)$ do *not* all represent the *same branch* of the algebraic function $\zeta(J)$.

Klein (1922) has shown that if we have found one root $\zeta_0 = \zeta_0(J)$ of the icosahedral equation then *all* the other roots of the equation can be expressed as fractional linear transformations of ζ_0. The detailed results are

$$\zeta = \zeta(J) = \varepsilon^{\mu}\zeta_0 \tag{42}$$

$$= -\varepsilon^{\mu}/\zeta_0 \tag{43}$$

$$= \varepsilon^{\mu}\left[\frac{(\varepsilon+\varepsilon^4)\zeta_0+\varepsilon^{\nu}}{\zeta_0-\varepsilon^{\nu}(\varepsilon+\varepsilon^4)}\right] \tag{44}$$

$$= -\varepsilon^{\mu}\left[\frac{\zeta_0-\varepsilon^{\nu}(\varepsilon+\varepsilon^4)}{(\varepsilon+\varepsilon^4)\zeta_0+\varepsilon^{\nu}}\right] \tag{45}$$

where

$$\varepsilon = \exp(2\pi i/5) \tag{46}$$

$\mu, \nu = 0, 1, 2, 3, 4$ and $\zeta_0 = \zeta_0(J)$. From these formulae we can now readily derive the following explicit expressions for the 12 roots $z = z(J)$ of the basic equation (10) with J real:

$$z_{0,\pm m} = z_c\left[\frac{\frac{1}{2}(\sqrt{5}-1)\zeta_0+\varepsilon^{\pm m}}{-\frac{1}{2}(\sqrt{5}+1)\zeta_0+\varepsilon^{\pm m}}\right]^5 \tag{47}$$

$z_{1,\pm m} = -1/z_{0,\pm m}$, $z_2 = \zeta_0^{-5}$, $z_3 = -1/z_2$, $z_4 = z_{0,0}$ and $z_5 = -1/z_4$, where $m = 1, 2$ and $\zeta_0 = \zeta_0(J)$ is the real root of the icosahedral equation. If the complex roots $z_{0,\pm1}(J)$ and $z_{1,\pm1}(J)$ are plotted for real values of J in the z plane one obtains a locus which is a complicated closed curve C_1. In a similar manner it is found that the complex roots $z_{0,\pm2}(J)$ and $z_{1,\pm2}(J)$ lie on a different closed curve C_2.

It is possible to consider ζ_0 to be a *parameter* for the plane curves C_1 and C_2 because for real J the function $\zeta_0(J)$ has real values in the interval

$$-\tfrac{1}{2}[(1-\sqrt{5})+\sqrt{2}(5-\sqrt{5})^{1/2}] < \zeta_0(J) \leq \tfrac{1}{2}[-(1+\sqrt{5})+\sqrt{2}(5+\sqrt{5})^{1/2}]. \tag{48}$$

We see, therefore, from equation (47) that the closed curves C_1 and C_2 can each be described in a piecewise manner by four *rational* parametric representations. A simplification of this result can be achieved by *formally* allowing the parameter ζ_0 to have *any* real value. In this manner we find that the curve C_1 has the *single* parametric representation

$$z = z_c\left[\frac{\frac{1}{2}(\sqrt{5}-1)\zeta_0+\varepsilon}{-\frac{1}{2}(\sqrt{5}+1)\zeta_0+\varepsilon}\right]^5 \tag{49}$$

where $-\infty < \zeta_0 < \infty$. For the curve C_2 we have the single representation

$$z = z_c \left[\frac{\frac{1}{2}(\sqrt{5}-1)\zeta_0 + \varepsilon^2}{-\frac{1}{2}(\sqrt{5}+1)\zeta_0 + \varepsilon^2} \right]^5 \tag{50}$$

where $-\infty < \zeta_0 < \infty$. It is clear from equations (49) and (50) that the curves C_1 and C_2 are both *rational* curves.

The cardioid drawn by Wood *et al* (1989) is part of the curve C_1 and has the representation (49) with the parameter ζ_0 in the intervals

$$-\tfrac{1}{4}[-(3+\sqrt{5}) + \sqrt{6}(5+\sqrt{5})^{1/2}] \leq \zeta_0 \leq 0 \tag{51}$$

$$\tfrac{1}{2}(\sqrt{5}-1) \leq \zeta_0 \leq \tfrac{1}{4}[(3-\sqrt{5}) + \sqrt{6}(5-\sqrt{5})^{1/2}]. \tag{52}$$

The other curve considered by Wood *et al* (1989) is part of C_2 and has the representation (50) with the parameter ζ_0 in the intervals

$$-\tfrac{1}{2}(\sqrt{5}+1) \leq \zeta_0 \leq -\tfrac{1}{4}[-(3-\sqrt{5}) + \sqrt{6}(5-\sqrt{5})^{1/2}] \tag{53}$$

$$-\tfrac{1}{4}[-(3+\sqrt{5}) + \sqrt{6}(5+\sqrt{5})^{1/2}] \leq \zeta_0 \leq 0. \tag{54}$$

It is interesting to note that the points where the curves C_1 and C_2 cross the real x axis are associated with parameter values ζ_0 which are zeros of the icosahedral polynomials $\zeta^5\Omega_1(\zeta^5)$, $\Omega_2(\zeta^5)$ and $\Omega_3(\zeta^5)$. One can also show that the positions of these crossing points are expressible in terms of the real zeros of the polynomials $\Omega_j(\zeta^5)$ $(j = 1, 2, 3)$. For example, the cardioid drawn by Wood *et al* (1989) crosses the negative x axis at

$$x = -\zeta_2^5 \tag{55}$$

where

$$\zeta_2 = \tfrac{1}{4}[(3-\sqrt{5}) + \sqrt{6}(5-\sqrt{5})^{1/2}] \tag{56}$$

is one of the zeros of the polynomial $\Omega_2(\zeta^5)$.

It can be shown by equating the imaginary part of equation (14) to zero that the cartesian coordinates $x = x(\zeta_0)$ and $y = y(\zeta_0)$ for both curves C_1 and C_2 satisfy a single polynomial equation of the type

$$P(x, y) \equiv \sum_{n=0}^{10} \sum_{m=0}^{20-2n} c_{nm} x^m y^{2n} = 0 \tag{57}$$

where c_{nm} are non-zero integers. From the parametric equations (49) and (50) one would expect that this equation is reducible to two independent polynomial equations $P_1(x, y) = 0$ and $P_2(x, y) = 0$ which are satisfied separately by the curves C_1 and C_2. These reduced equations will have coefficients which involve *irrational* numbers such as $\sqrt{5}$.

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