The Hard Hexagon Partition Function for Complex Fugacity

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Baxter computed the fugacity \( z \) and the partition function per site

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\kappa_{\pm}(z) = \lim_{L_h \to \infty} \lambda_{\text{max}}(z; L_h)^{1/L_h}
\]

for positive \( z \) terms of an auxiliary variable \( x \) using the functions

\[
G(x) = \prod_{n=1}^{\infty} \frac{1}{(1 - x^{5n-4})(1 - x^{5n-1})},
\]

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H(x) = \prod_{n=1}^{\infty} \frac{1}{(1 - x^{5n-3})(1 - x^{5n-2})},
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Q(x) = \prod_{n=1}^{\infty} (1 - x^n).
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Regions \( 0 \leq z \leq z_c < \infty \) with \( z_c = \left( \frac{11 + 5\sqrt{5}}{2} \right) = 11.090168 \cdots \)
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Partition functions per site

For high density where $0 < z^{-1} < z_c^{-1}$ the results are

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z = \frac{1}{x} \left( \frac{G(x)}{H(x)} \right)^5; \quad \kappa_+ = \frac{1}{x^{1/3}} \frac{G^3(x) Q^2(x^5)}{H^2(x)} \prod_{n=1}^{\infty} \frac{(1 - x^{3n-2})(1 - x^{3n-1})}{(1 - x^{3n})^2}.
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For low density where $0 \leq z < z_c$

$$z = -x \left( \frac{H(x)}{G(x)} \right)^5; \quad \kappa_- = \frac{H^3(x) Q^2(x^5)}{G^2(x)} \prod_{n=1}^{\infty} \frac{(1 - x^{6n-4})(1 - x^{6n-3})^2(1 - x^{6n-2})}{(1 - x^{6n-5})(1 - x^{6n-1})(1 - x^{6n})^2}.$$
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$\kappa_{\pm}(z)$ have singularities at $z_c$, $z_d = -1/z_c$ and $\infty$. 
The equimodular curve $|\kappa_-(z)| = |\kappa_+(z)|$

If the two eigenvalues $\kappa_-(z)$ and $\kappa_+(z)$ suffice to describe the partition function in the entire complex $z$ plane then there will be zeros on the equimodular curve $|\kappa_-(z)| = |\kappa_+(z)|$. 
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The partition function on a lattice with $L_v$ rows and $L_h$ columns is

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where $g(N)$ is the number of allowed configurations with $N$ particles.
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Numerically we compute the partition function using a transfer matrix algorithm to build the finite lattice site-by-site.
Hard hexagon partition function zeros
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15x15

18x18
Hard hexagon partition function zeros
Hard hexagon partition function zeros

Iwan Jensen (University of Melbourne)

ANZAMP 2013 7 / 19
Hard hexagon partition function zeros
1. There is a 'necklace' on the left side. Baxter's solution does not tell the whole story.

2. Starting with $30\times30$ zeros start to appear in the necklace and separated regions begin to be apparent.

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Hard hexagon partition function zeros

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An alternative representation of the partition function on a finite lattice is given in terms of the eigenvalues of the transfer matrix $T_{Lh}(z)$. When the transfer matrix is diagonalizable the partition function may be written in terms of the eigenvalues $\lambda_k$ and eigenvectors $v_k$ of the transfer matrix $T_{Lh}(z)$ as

$$Z_{Lh}(z) = \sum_k \lambda_k v_k(z; Lh)c_k$$

where $c_k = (v_B \cdot v_k)(v_k \cdot v'_B)$.

and $v_B$ and $v'_B$ are suitable vectors for the boundary conditions on rows 1 and $L$. 
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On this curve $\lambda_1(z; L_h)/\lambda_2(z; L_h) = e^{i\phi(z)}$ with $\phi(z)$ real.
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The density of zeros on this curve is proportional to $d\phi(z)/dz$. 

Calculating Equimodular Curves

We don’t actually calculate the eigenvalues directly from $T_{Lh}(z)$. We use iterative diagonalisation methods where one studies not $T$ itself but rather its repeated action on a suitable set of vectors. We work with vectors $T^nw$ produced by the power method. An iterative scheme that works well even in the presence of complex and degenerate eigenvalues is known as Arnoldi’s method. We make use of the public domain software package ARPACK implementing Arnoldi’s method with suitable subtle stopping criteria. The ARPACK package allows one to calculate eigenvalues (and eigenvectors) based on various criteria, including the one relevant to our calculations, namely the eigenvalues of largest modulus. We developed routines to automatically trace equimodular curves.
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Hard Hexagons

ANZAMP 2013  13 / 19
Hard hexagon equimodular curves

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Dominant eigenvalue crossings in red; $|\kappa_-(z)| = |\kappa_+(z)|$ in black.
Just for fun. Some Hard Squares results

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Hard Hexagons

ANZAMP 2013 15 / 19
Just for fun. Some Hard Squares results

26x26
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26x26

26x52
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26x26

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26x78
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According to finite-size scaling the free energy per site corresponding to the $j$-th eigenvalue of the transfer matrix has the scaling form

$$\frac{1}{L} f_j \left( |z - z_c| L^y, u L^{-|y'|} \right),$$

where $z_c$ is the critical point, $y$ is the leading relevant eigenvalue and $u$ is the coupling to an irrelevant operator with eigenvalue $y' < 0$, which implies at leading order that

$$|z - z_c| = AL^{-y} + BuL^{-y-|y'|} + \ldots ,$$

where $A$ and $B$ are non-universal constants.
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where $A$ and $B$ are non-universal constants.

To higher orders, terms on the RHS involve powers of $L^{-1}$ that can be any non-zero linear combination of $y$ and $|y'|$ with non-negative integer coefficients.
Finite-size behaviour at $z_c$

The critical point $z_c > 0$ of hard hexagons is known to be in the same universality class as the three-state ferromagnetic Potts model.
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Our numerical analysis of $|z_c(L)| - z_c$ for $L$ up to 39 gives good evidence for the scaling form

$$|z_c(L)| - z_c = a_0 L^{-6/5} + a_1 L^{-2} + a_2 L^{-14/5} + \ldots$$
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The powers of $L^{-1}$ appearing on the right-hand side can be identified with $y$, $y + |y'|$ and $y + 2|y'|$. 
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This is compatible with the above general result.
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However, note that powers such as $y + 1 = 11/5$ and $2y = 12/5$, which are possible in principle, are not observed numerically.
Finite-size behaviour at $z_d$

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Our numerical analysis of $|z_d(L) - z_d|$ gives strong evidence for the scaling form

$$|z_d(L) - z_d| = b_0 L^{-12/5} + b_1 L^{-17/5} + b_2 L^{-22/5} + \ldots$$

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The powers of $L^{-1}$ on the right-hand side can be identified with $y$, $y + 1$ and $y + 2$.

The integer shifts can be related to descendent operators in the CFT, since $|y'|$ is a positive integer for descendents of the identity operator.