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# Hard hexagons: interfacial tension and correlation length

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Abstract. Functional equations are derived for the eigenvalues of the row-to-row transfer matrix of the generalised hard hexagon model. These equations are exact for a lattice with N columns and are solved in the limit  $N \rightarrow \infty$ . The partition function per site is thereby rederived without the previous analyticity assumptions. We are also able to calculate the interfacial tension and the correlation length; the associated critical exponents are  $\mu = \nu = \nu' = \frac{5}{6}$  in agreement with the scaling relations.

## 1. Introduction

In previous papers (Baxter 1980a, 1981a) it has been shown that the hard hexagon model (triangular lattice gas with nearest-neighbour exclusion) can be solved exactly. More specifically, the free energy has been obtained using a matrix inversion trick and the order parameters (sublattice densities) have been obtained using corner transfer matrices. These techniques apply equally to the eight-vertex model (Baxter 1980b, 1981b, Shankar 1981). However, for the eight-vertex model (Baxter 1972), one can also obtain tractable equations for the eigenvalues of the row-to-row transfer matrix. It is thus possible to calculate the interfacial tension (Baxter 1973) and correlation length (Johnson *et al* 1973). It is clearly desirable to carry out such a program for hard hexagons. In this paper we indicate how this is done and give the main results. In particular, we find that the critical exponents are

$$\mu = \nu = \nu' = \frac{5}{6}.\tag{1.1}$$

Since  $\alpha = \alpha' = \frac{1}{3}$ , the scaling relations

$$\alpha = \alpha'$$
  $\nu = \nu' = (\mu + \nu)/d = (2 - \alpha)/d$  (1.2)

(where d = 2 is the dimensionality) are therefore satisfied.

The layout of the paper is as follows. In the next section we define the generalised hard hexagon model. In § 3 we derive an exact functional equation satisfied by the transfer matrix. We write this in ways appropriate to the various ordered and disordered regimes. In §§ 4 and 5 we consider regimes I and II (Baxter 1980a), respectively; these include the pure hard hexagon model as a limiting case. We outline the method for solving the transfer matrix equations and give the results. The results for regimes III and IV, and further details of the calculation, will be given elsewhere.

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## 2. Generalised hard hexagon model

The hard hexagon model can be regarded as a special case of a hard square lattice gas with diagonal interactions. We therefore begin by considering a square lattice of P rows and N columns with toroidal boundary conditions. To each site *i* of the lattice we assign an occupation number  $\sigma_i$ ; if the site *i* is empty  $\sigma_i = 0$ , if the site *i* is full  $\sigma_i = 1$ . The partition function for this lattice of NP sites is then

$$Z = \sum_{\sigma} \prod_{(i,j,k,l)} W(\sigma_i, \sigma_j, \sigma_k, \sigma_l)$$
(2.1)

where the sum is over all values of the occupation numbers and the product is over all faces of the lattice (i, j, k, l) being the four sites round a face, starting at the bottom-left and going anticlockwise). The function W(a, b, c, d) is the Boltzmann weight of the interactions within a face. It is of the form

$$W(a, b, c, d) = \begin{cases} mz^{(a+b+c+d)/4} e^{Lac+Mbd} t^{-a+b-c+d} & \text{if } ab = bc = cd = da = 0\\ 0 & \text{otherwise.} \end{cases}$$
(2.2)

Here the activity z > 0 has been shared out between adjacent faces, L and M are the diagonal interactions, m is a trivial normalisation factor and t is a parameter that cancels out of the partition function and the transfer matrix.

Let  $\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \dots, \sigma_N\}$  be the configuration of a row of sites with nearestneighbour exclusion so that  $\sigma_j \sigma_{j+1} = 0, j = 1, 2, \dots, N$ . The number of such configurations is then

$$A_{N} = \left[\frac{1}{2}(1+\sqrt{5})\right]^{N} + \left[\frac{1}{2}(1-\sqrt{5})\right]^{N}.$$
(2.3)

If  $\sigma$  and  $\sigma'$  are the configurations of two successive rows the (row-to-row) transfer matrix V is defined to be the  $A_N \times A_N$  matrix with elements

$$V_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = \prod_{j=1}^{N} W(\boldsymbol{\sigma}_{j}, \boldsymbol{\sigma}_{j+1}, \boldsymbol{\sigma}_{j+1}', \boldsymbol{\sigma}_{j}').$$
(2.4)

The partition function can then be written as

$$Z = \sum_{\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \dots, \boldsymbol{\sigma}_P} V_{\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2} V_{\boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3} \dots V_{\boldsymbol{\sigma}_P, \boldsymbol{\sigma}_1} = \operatorname{Tr} \boldsymbol{V}^P$$
(2.5)

where the sum is over all row configurations and Tr denotes trace. Unless L = M, the matrix V is not symmetric. Its eigenvalues will therefore generally be complex. However, since V is non-negative the Perron-Frobenius theorem guarantees that the eigenvalue  $V_0$  of largest modulus is real and non-degenerate. The partition function per site is therefore given by

$$\kappa = \lim_{N \to \infty} \lim_{P \to \infty} Z^{1/NP} = \lim_{N \to \infty} V_0^{1/N}.$$
(2.6)

We wish to consider models whose transfer matrices commute. Following Baxter (1980a), we restrict our attention to models satisfying the constraint

$$z = (1 - e^{-L})(1 - e^{-M})/(e^{L+M} - e^{L} - e^{M}).$$
(2.7)

It can then be shown that if two models, each satisfying this constraint, differ in their

values of z, L, M, but have the same value of

$$\Delta = z^{-1/2} (1 - z \ e^{L+M}) \tag{2.8}$$

then their transfer matrices commute.

Eliminating z between (2.7) and (2.8) gives a symmetric biquadratic relation between  $e^{L}$  and  $e^{M}$ . This is naturally parametrised in terms of elliptic functions. Explicitly, we use the parametrisation

$$e^{L} = \theta(\lambda)\theta(2\lambda + u)\theta(2\lambda - u)/[\theta(2\lambda)\theta^{2}(u)]$$
  

$$e^{M} = \theta(\lambda)\theta(3\lambda - u)\theta(\lambda + u)/[\theta(2\lambda)\theta^{2}(\lambda - u)]$$
(2.9)

$$z = \theta^{3}(2\lambda)\theta^{2}(u)\theta^{2}(\lambda-u)/[\theta^{3}(\lambda)\theta^{4}(2\lambda+u)] \qquad \Delta^{2} = [\theta(\lambda)/\theta(2\lambda)]^{5}$$
(2.10)

where  $\lambda = \pi/5, -\lambda < u < 2\lambda$  and

$$\theta(u) = \theta(u, q^2) = \sin u \prod_{n=1}^{\infty} (1 - q^{2n} e^{2iu})(1 - q^{2n} e^{-2iu})(1 - q^{2n})$$
(2.11)

is (apart from an irrelevant factor) a standard elliptic theta function of nome  $q^2$  with  $-1 < q^2 < 1$ . If we choose *m* and *t* in (2.2) appropriately, the Boltzmann weights of the allowed configurations round a face can now be written as

$$\omega_{1}(u) = W(0000) = \theta(2\lambda + u)/\theta(2\lambda)$$
  

$$\omega_{2}(u) = W(1000) = W(0010) = \pm \theta(u)/[\theta(\lambda)\theta(2\lambda)]^{1/2}$$
  

$$\omega_{3}(u) = W(0100) = W(0001) = \theta(\lambda - u)/\theta(\lambda)$$
  

$$\omega_{4}(u) = W(1010) = \theta(2\lambda - u)/\theta(2\lambda)$$
  

$$\omega_{5}(u) = W(0101) = \theta(\lambda + u)/\theta(\lambda).$$
  
(2.12)

Regarding  $q^2$  as fixed and u as a variable we see that (2.4) and (2.12) define a one-parameter family of commuting transfer matrices.

We end this section with two remarks. First, in the next section we will need to distinguish between the cases  $q^2 < 0$  and  $q^2 > 0$ . This leads us to consider four distinct physical regimes (phases):

Regime I (disordered)	$-1 < q^2 < 0,$	$-\lambda < u < 0$	
Regime II (triangular ordered)	$0 < q^2 < 1,  -\lambda < u < 0$	(0.12)	
Regime III (disordered)	$0 < q^2 < 1,$	$0 < u < \lambda$	(2.13)
Regime IV (square ordered)	$-1 < q^2 < 0,$	$0 < u < \lambda$ .	

From (2.10) and (2.11) it follows that the borderline case  $q^2 = 0$  occurs on lines in the (L, M) plane given by

$$\Delta = \pm \Delta_{\rm c}, \qquad \Delta_{\rm c}^{-2} = \left[\frac{1}{2}(1+\sqrt{5})\right]^5. \tag{2.14}$$

As we shall see, these lines are in fact the critical lines (phase boundaries) of the model. The second remark is that, in the above parametrisation, the hard hexagon model  $(L = 0, M = -\infty)$  clearly corresponds to the limit  $u \rightarrow -\lambda$ . Thus only regimes I and II are relevant to the solution of the hard hexagon model.

## 3. Transfer matrix equations

#### 3.1. Derivation

To derive the transfer matrix equations we start by looking at the matrix product of the transfer matrices V = V(u) and  $V' = V(u + \lambda)$ . Using (2.4) we find

$$[\boldsymbol{V}\boldsymbol{V}']_{\boldsymbol{\sigma},\boldsymbol{\sigma}'} = \sum_{\tau_1,\tau_2,\dots,\tau_N=0,1} \prod_{j=1}^N W(\sigma_j,\sigma_{j+1},\tau_{j+1},\tau_j) W'(\tau_j,\tau_{j+1},\sigma_{j+1}',\sigma_j')$$
  
= Tr  $\boldsymbol{R}(\sigma_1,\sigma_2,\sigma_2',\sigma_1') \boldsymbol{R}(\sigma_2,\sigma_3,\sigma_3',\sigma_2') \dots \boldsymbol{R}(\sigma_N,\sigma_1,\sigma_1',\sigma_N')$  (3.1)

where the nine matrices  $\boldsymbol{R}(\sigma_1, \sigma_2, \sigma_2', \sigma_1')$  have elements

$$[R(\sigma_1, \sigma_2, \sigma'_2, \sigma'_1)]_{\tau_1, \tau_2} = W(\sigma_1, \sigma_2, \tau_2, \tau_1)W'(\tau_1, \tau_2, \sigma'_2, \sigma'_1)$$
(3.2)

and  $W'(\tau_1, \tau_2, \sigma'_2, \sigma'_1)$  is given by (2.12) with u replaced by  $u + \lambda$ .

If  $\sigma_i = \sigma'_i = 0$ ,  $\tau_i$  can assume the values 0 or 1 and the corresponding **R** matrices have two rows or columns. Otherwise, we must have  $\tau_i = 0$  and the corresponding **R** matrices have one row or column. Thus **R**(0000) is a 2×2 matrix; all the other **R** matrices are row vectors (1×2), column vectors (2×1) or scalars (1×1). We find that **R**(0000) has a right eigenvector **x** and a left eigenvector  $\mathbf{y}^{\mathrm{T}}$  which are independent of *u* and orthogonal. The corresponding eigenvalues are  $\theta(\lambda - u)\theta(\lambda + u)/\theta^2(\lambda)$  and  $\theta^2(u)/\theta(\lambda)\theta(2\lambda)$ . We find further than **R**(0110) is proportional to **x** and that **R**(1000) and **R**(0001) are proportional to  $\mathbf{y}^{\mathrm{T}}$ .

Because of the periodic boundary conditions, the above observations suffice to show that the non-zero elements of  $[VV']_{\sigma,\sigma'}$  fall into two categories: either  $\sigma_j = \sigma'_j$  for all j (these are the diagonal elements), or  $\sigma_j \sigma'_j = 0$  for all j. In the latter case, examination of the matrix elements shows that they are in fact the matrix elements of  $[\theta(u)/\theta(\lambda)]^N V(u-2\lambda)$ . In this way we obtain the transfer matrix equation

$$\mathbf{V}(u)\,\mathbf{V}(u+\lambda) = \left[\theta(\lambda-u)\theta(\lambda+u)/\theta^2(\lambda)\right]^N \mathbf{I} + \left[\theta(u)/\theta(\lambda)\right]^N \mathbf{V}(u-2\lambda) \tag{3.3}$$

where I is the identity matrix.

We have already noticed that V(u) is a one-parameter family of commuting transfer matrices. Interchanging L and M in (2.7) and (2.8), we see that each V in the family is normal, that is, commutes with its transpose. The matrices are therefore simultaneously diagonalisable and have in common a complete set of orthonormal eigenvectors independent of u. If V(u) is an eigenvalue of V(u), associated with a particular eigenvector, it follows that V(u) must satisfy the functional equation given by (3.3). To simplify the form of this equation we introduce the 'dimensionless' transfer matrix

$$\boldsymbol{T}(u) = \left(-\frac{\omega_1(u)}{\omega_4(u)\omega_5(u)}\right)^N \boldsymbol{V}(u)$$
(3.4)

with eigenvalues T(u). Putting this in (3.3) and using (2.12) then gives the eigenvalue equation

$$T(u)T(u+\lambda) = 1 + T(u-2\lambda).$$
(3.5)

Using the identity  $\theta(u + \pi) = -\theta(u)$ , we also obtain the periodicity relation

$$T(u+5\lambda) = T(u). \tag{3.6}$$

## 3.2. Conjugate modulus parametrisations

Rather than solve the transfer matrix equation (3.5) directly it is convenient to transform to the conjugate modulus forms. These forms differ in the various physical regimes but are better suited to our purposes. If -1 < x < 1, we define

$$f(w, x) = \prod_{n=1}^{\infty} (1 - x^{n-1}w)(1 - x^n w^{-1})(1 - x^n)$$
(3.7)

and adopt the convention

$$f(w) = f(w, x^{5}).$$
 (3.8)

The function f(w, x) is then related to the elliptic theta function  $\theta(u, q^2)$  by the conjugate modulus identities

$$\theta(u, e^{-\varepsilon}) = \frac{1}{2} \left(\frac{2\pi}{\varepsilon}\right)^{1/2} \exp\left(\frac{\varepsilon}{8} - \frac{\pi^2}{2\varepsilon} + \frac{2u(\pi - u)}{\varepsilon}\right) f(e^{-4\pi u/\varepsilon}, e^{-4\pi^2/\varepsilon})$$
(3.9*a*)

$$\theta(u, -e^{-\varepsilon}) = -\frac{1}{2} \left(\frac{\pi}{\varepsilon}\right)^{1/2} \exp\left(\frac{\varepsilon}{8} - \frac{\pi^2}{8\varepsilon} - \frac{u(2u+\pi)}{\varepsilon}\right) f(e^{2\pi u/\varepsilon}, -e^{-\pi^2/\varepsilon}).$$
(3.9b)

The first equation applies when  $q^2 > 0$ , the second when  $q^2 < 0$ .

Let us now define the new parameters x and w by

I and IV  $x = -e^{-\pi^2/5\varepsilon}$   $w = e^{2\pi u/\varepsilon}$   $q^2 = -e^{-\varepsilon}$  (3.10*a*) II and III  $x = e^{-4\pi^2/5\varepsilon}$   $w = e^{-4\pi u/\varepsilon}$   $q^2 = e^{-\varepsilon}$ . (3.10*b*)

Then using the identities (3.9), the parameters m and t in (2.2) can be chosen so that in regimes I and IV:

$$\omega_{1}(w) = f(xw)/f(x) \qquad \qquad \omega_{2}(w) = \pm (-x)^{1/2} f(w)/[f(x)f(x^{2})]^{1/2}$$
  

$$\omega_{3}(w) = f(x^{2}w)/f(x^{2}) \qquad \qquad \omega_{4}(w) = wf(xw^{-1})/f(x) \qquad (3.11)$$
  

$$\omega_{5}(w) = f(x^{2}w^{-1})/f(x^{2}) \qquad \qquad \Delta^{2} = -x[f(x^{2})/f(x)]^{5}.$$

Here x and w lie in the ranges

Regime I 
$$-1 < x < 0, \quad x^2 < w < 1$$
  
Regime IV  $-1 < x < 0, \quad 1 < w < x^{-2}.$ 
(3.12)

In conjugate modulus form the equations (3.4)-(3.6) become

$$T(w)T(x^{3}w) = 1 + T(x^{4}w)$$
(3.13a)

$$T(x^5w) = T(w) \tag{3.13b}$$

$$T(w) = \left(-\frac{f(x^2)f(xw)}{wf(xw^{-1})f(x^2w^{-1})}\right)^N V(w).$$
(3.13c)

Likewise, in regimes II and III, we obtain the alternative parametrisation

$$\omega_{1}(w) = f(x^{2}w)/f(x^{2}) \qquad \omega_{2}(w) = \pm x^{1/2}f(w)/[f(x)f(x^{2})]^{1/2}$$
  

$$\omega_{3}(w) = f(xw^{-1})/f(x) \qquad \omega_{4}(w) = wf(x^{2}w^{-1})/f(x^{2}) \qquad (3.14)$$
  

$$\omega_{5}(w) = w^{-1}f(xw)/f(x) \qquad \Delta^{2} = x[f(x)/f(x^{2})]^{5}.$$

This time x and w lie in the ranges

**Regime II** 
$$0 < x < 1, 1 < w < x^{-1}$$
 (3.15*a*)

**Regime III** 
$$0 < x < 1, x < w < 1.$$
 (3.15b)

With this parametrisation the equations (3.4)-(3.6) become

$$T(w)T(xw) = 1 + T(x^{3}w)$$
(3.16a)

$$T(x^{5}w) = T(w)$$
 (3.16b)

$$\Gamma(w) = \left(-\frac{f(x)f(x^2w)}{f(xw)f(x^2w^{-1})}\right)^N V(w).$$
(3.16c)

## 3.3. Analyticity and zeros

So far, we have used the algebraic properties of the transfer matrix V(w) to obtain functional equations for its eigenvalues V(w). To solve these equations we now exploit the analytic properties of V(w). From (3.11) and (3.14) we see that the matrix elements of V(w) are analytic within the annulus  $0 < |w| < \infty$  in the complex w plane. Since the eigenvectors of V(w) are independent of w it follows, at least for finite N, that the eigenvalues V(w) are also analytic in the annulus  $0 < |w| < \infty$ . Using this fact and periodicity it can be shown (by applying the residue theorem to the integral of the logarithmic derivative of V(w) round a period annulus) that any eigenvalue V(w) must be of the form

$$V(w) = Rw^{n} \prod_{j=1}^{N} f(w/w_{j}).$$
(3.17)

Here *n* is an integer, *R* is complex and  $w_1, w_2, \ldots, w_N$  are the *N* zeros of V(w) within a period annulus such as  $1 \le |w| < |x|^{-5}$ . Using periodicity and the identity  $f(x^5w) = -w^{-1}f(w)$ , we also obtain the exact relation

$$\prod_{j=1}^{N} w_j = \begin{cases} x^{-5n-N} & \text{regimes I, IV} \\ x^{-5n-2N} & \text{regimes II, III.} \end{cases}$$
(3.18)

From (3.17) it is clear that the eigenvalues V(w) are determined by their zeros in the complex w plane, or more precisely, by the N + 1 complex numbers  $R, w_1, w_2, \ldots, w_N$ . From (3.18), however, only N of these unknowns are independent. In principle, these can be determined by solving the N equations

$$T(x^{p}w_{i}) = -1$$
  $j = 1, 2, ..., N$  (3.19)

where p = 1 or 4 in regimes I and IV, and p = 2 or 3 in regimes II and III. These equations are analogous to the Bethe ansatz equations for the ice-type models (Lieb and Wu 1972, equation (147)) and are readily obtained by choosing w in the transfer matrix equations (3.13a) and (3.16a) so that the left side vanishes.

In the limit of N large, we will see that most of the zeros of the largest eigenvalues are densely distributed on circles in the complex w plane. In this limit, it is then possible to calculate the largest eigenvalues without precisely locating all their zeros. This we do for regimes I and II in the next two sections. For hard hexagons, we are interested in the limits  $w \to x^2$  in regime I and  $w \to x^{-1}$  in regime II.

## 4. Regime I

#### 4.1. Largest eigenvalues

We wish to solve the transfer matrix equation (3.13a) for the largest eigenvalues in regime I. This equation, however, does not distinguish between regimes I and IV; its solutions will be eigenvalues in both regimes. On the other hand, the *largest* eigenvalues in regimes I and IV will be different. This is because the eigenvalues cross at the boundary w = 1. At this point, V(w) becomes the shift operator and all the eigenvalues are unimodular.

When N is large, there are many solutions of (3.13a). To select out those eigenvalues that are largest in regime I, we appeal to perturbation expansions. Perturbation about the vacuum state (the  $x \rightarrow 0$  – limit in regime I) suggests that for the largest eigenvalues

$$V(w) = O(1) \text{ as } N \to \infty$$
  $x^2 < |w| < 1.$  (4.1)

We therefore look for solutions with this property. Using (4.1) in (3.13) we find that for large N

$$|T(x^{4}w)| = O(|x|^{-eN}) \gg 1 \qquad x^{4} < |w| < |x|$$
  
$$|T(x^{4}w)| = O(|x|^{eN}) \ll 1 \qquad |x| < |w| < |x|^{-1} \qquad (4.2)$$

with  $\varepsilon > 0$ . For large N, this tells us that one of the terms on the right side of (3.13a) is exponentially larger (in modulus) than the other.

By keeping just the dominant term it is now possible to locate the zeros of V(w) in the limit  $N \to \infty$ . We find that zeros are only allowed on the circles  $|w| = |x|^{-1}$ , |x|,  $x^2$  (or more precisely  $|w| = |x|^{5n-1}$ ,  $|x|^{5n+1}$ ,  $|x|^{5n+2}$  by periodicity). Moreover, if |a| = 1 and w = ax is a zero, then so is  $w = ax^2$  and vice versa, so these zeros appear in pairs. From (3.17), it follows that for large N, the eigenvalues must be of the form

$$V_{r}(w) = Rw^{r} \prod_{j=1}^{r} f(x^{3}w/a_{j})f(x^{4}w/a_{j}) \prod_{k=1}^{N-2r} f(xw/b_{k})$$
(4.3)

where r is a non-negative integer not greater than  $\frac{1}{2}N$  and the  $a_j$  and  $b_k$  are complex numbers which depend on x and are unimodular in the limit  $N \to \infty$ . The leading power of w is fixed by periodicity, that is, by (3.18). Although we have exhibited the dependence of V(w) on r, there are, in general, many eigenvalues corresponding to a given value of r. The index r labels bands of eigenvalues.

Define L(w) by

$$T_r(w) = w^{r-N} L(w) \prod_{j=1}^r (1 - xa_j w^{-1})(1 - x^2 a_j w^{-1})/(1 - x w^{-1})^N (1 - x^2 w^{-1})^N$$
(4.4)

with  $T_r(w)$  related to  $V_r(w)$  by (3.13c). From (4.3) and (3.7), L(w) is analytic and non-zcro in the annulus  $x^4 < |w| < |x|^{-1}$  and  $\ln L(w)$  is also analytic therein. Now consider the smaller annulus  $1 < |w| < |x|^{-1}$ . In this annulus the second term on the right side of (3.13a) is dominant (i.e. for large N it is exponentially larger than the first), so the first term can be ignored in the limit  $N \to \infty$ . Taking logarithms, using (4.4), Laurent expanding and equating coefficients, we can solve for  $\ln L(w)$ . We find that

$$T_r(w) = \phi^N(w) \prod_{j=1}^r \phi(a_j w^{-1}) \qquad x^4 < |w| < |x|^{-1}$$
(4.5)

where

$$\phi(w) = -w^{-1} \frac{f(xw, x^6)f(x^2w, x^6)}{f(xw^{-1}, x^6)f(x^2w^{-1}, x^6)}.$$
(4.6)

If we set  $w = a_i x$  in the transfer matrix equation (3.13*a*) the left-hand side vanishes and

$$1 + T_r(a_i) = 0. (4.7)$$

That is, the  $a_i$  are solutions of the equations

$$\phi^{N}(a_{i}) = -\prod_{j=1}^{r} \phi(a_{i}/a_{j}) \qquad i = 1, 2, \dots, r.$$
(4.8)

Since  $|\phi'(w)| = 1$  when |w| = 1, these equations are consistent with the requirement that the  $a_i$  be unimodular. It is also interesting to note the similarity in form to the Bethe ansatz equations.

For r=0, the transfer matrix V(w) has just one eigenvalue  $V_0(w)$  given by  $T_0(w) = \phi^N(w)$ . In the physical regime  $x^2 \le w \le 1$ , this is real and is the eigenvalue of largest modulus. From (2.6) and (3.4), it follows that the partition function per site is

$$\kappa(w) = -\omega_4(w)\omega_5(w)\phi(w)/\omega_1(w) \tag{4.9}$$

where  $\omega_1(w)$ ,  $\omega_4(w)$  and  $\omega_5(w)$  are given by (3.11). This agrees with the result (Baxter 1980a) previously obtained by the matrix inversion trick.

For each positive integer r, (4.5) and (4.8) give a band of complex eigenvalues. Since  $|\phi(w^{-1})| < 1$ , for  $x^3 < |w| < 1$ , there will be a gap

$$V_1(w)/V_0(w) = T_1(w)/T_0(w) = \phi(a_1w^{-1})$$
 (4.10)

between the largest and next-largest eigenvalues. For r = 1, (4.8) becomes

$$\phi^{N}(a_{1}) = 1. \tag{4.11}$$

The solutions of this equation give a band of N complex next-largest eigenvalues. For r = 2, there is a band of  $\frac{1}{2}N(N-3)$  complex next-next-largest eigenvalues and so on. We shall assume, as seems reasonable from small x expansions, that in the limit  $N \to \infty$ , the solutions of (4.8) form continuous distributions on the circles  $|a_1| = 1$ ,  $|a_2| = 1$ , etc with densities  $\rho(a_1)$ ,  $\rho(a_1, a_2)$ , etc.

### 4.2. Correlation length

We are now in a position to calculate the correlation length in the physical regime  $x^2 < w < 1$ . Since there is a gap between the largest and next-largest eigenvalues; we expect the correlation between occupation numbers at two sites, in the same column but separated by l rows, to decay exponentially for large l. By standard transfer matrix arguments (see, for example, Baxter 1981b), the pair correlation function is

$$\langle \sigma_0 \sigma_l \rangle = \sum_r \sum_{\boldsymbol{a}_r} c_{r,\boldsymbol{a}_r} [V_{r,\boldsymbol{a}_r}(w) / V_0(w)]^l$$
(4.12)

where the sum is over all eigenvalues  $V_{r,a_r}(w)$  with  $a_r = (a_1, a_2, \ldots, a_r)$  a multi-index labelling the eigenvalues in the *r*th band. The coefficients  $c_{r,a_r}$  are independent of *l* and *w* and depend only on the eigenvectors. In the limit  $N \rightarrow \infty$ , we assume that these coefficients become continuous and absorb the function  $c_r(a_1, a_2, \ldots, a_r)$  into the

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density  $\rho(a_1, a_2, \ldots, a_r)$ . Each sum over  $a_r$  in (4.12), with  $r \ge 1$ , can then be replaced by an *r*-fold integral. For *l* large, only the next-largest band of eigenvalues is expected to contribute to the leading order asymptotic behaviour of the correlations. Discarding the bands with  $r \ge 2$  and using (4.10), we find for large *l* 

$$\langle \sigma_0 \sigma_l \rangle - \langle \sigma_0 \rangle \langle \sigma_l \rangle \sim \frac{1}{2\pi i} \oint_{|a_1|=1} \frac{\mathrm{d}a_1}{a_1} \rho(a_1) \phi^l(a_1 w^{-1}). \tag{4.13}$$

In the limit  $l \rightarrow \infty$  this integral can be evaluated by steepest descents. Because of the symmetry

$$\phi(x^3 w) = \phi(w^{-1}) \tag{4.14}$$

 $|\phi(w)|$  has saddle points at

$$w = \pm w_s$$
  $w_s = i|x|^{-3/2}$ . (4.15)

Moreover, if we assume that  $\rho(a_1)$  is analytic in the annulus  $|x|^{1/2} < |a_1| < |x|^{-3/2}$ , the contour  $|a_1| = 1$  in (4.13) is equivalent to the contour  $|a_1| = |x|^{-3/2}w$ . Since the contributions from the two saddle points on this contour are complex conjugates we find that for large l

$$\langle \sigma_0 \sigma_l \rangle - \langle \sigma_0 \rangle \langle \sigma_l \rangle \sim A \, \mathrm{e}^{-l\xi^{-1}} \cos(l\eta + \delta)$$

$$\tag{4.16}$$

where

$$\phi(w_s) = e^{-\xi^{-1} + i\eta} \tag{4.17}$$

and A and  $\delta$  are real and related to  $\rho(w_s w)$ . Hence the correlation length  $\xi$  is independent of w, as is implied by the commutation properties of the transfer matrices, and is given by

$$-\xi^{-1} = \ln|\phi(\mathbf{i}|x|^{-3/2})|. \tag{4.18}$$

As we approach criticality (i.e. let  $x \rightarrow 1-$ ) the correlation length  $\xi$  diverges and  $\eta \rightarrow \frac{2}{3}\pi$  reflecting the onset of triangular ordering. In the original parametrisation (see (3.9) and (3.10)), we find that near criticality

$$\xi \sim \frac{1}{2\sqrt{3}} (-q^2)^{-5/6} \qquad q^2 \to 0-.$$
 (4.19)

Hence the correlation exponent is

$$\nu = 5/6.$$
 (4.20)

## 5. Regime II

#### 5.1. Largest eigenvalues

Perturbation expansions about the triangular ordered state (the  $x \rightarrow 0+$  limit) suggest that for the largest eigenvalues in regime II

$$V(w) = O(w^{N/3}) \text{ as } N \to \infty$$
  $1 < |w| < x^{-2}$ . (5.1)

Using this in the transfer matrix equation (3.16), we find for large N

$$|T(x^{3}w)| = O(x^{-\epsilon N}) \gg 1 \qquad x^{2} < |w| < x^{1/2} \qquad x^{-1/2} < |w| < x^{-2} |T(x^{3}w)| = O(x^{\epsilon N}) \ll 1 \qquad x^{3} < |w| < x^{2} \qquad x^{1/2} < |w| < x^{-1/2}$$
(5.2)

with  $\varepsilon > 0$ .

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If we retain only the dominant term on the right-hand side of (3.16a) for large N, we find that V(w) can only have zeros on the circles  $|w| = x^{-2}$ ,  $x^{-1}$ ,  $x^{-1/2}$ ,  $x^{1/2}$ ,  $x^{3/2}$ ,  $x^{2}$  with the zeros  $w = ax^{-1}$ ,  $ax^{2}$  and  $w = bx^{-1/2}$ ,  $bx^{3/2}$  appearing in pairs. It follows, from (3.17), that the largest eigenvalues for large N must be of the form

$$V_{p,r}(w) = \mathbf{R}w^{n} \prod_{i=1}^{p} f(xw/a_{i})f(x^{3}w/a_{i})$$

$$\times \prod_{j=1}^{r} f(x^{1/2}w/b_{j})f(x^{7/2}w/b_{j}) \prod_{k=1}^{s} f(x^{2}w/c_{k}) \prod_{l=1}^{r} f(x^{9/2}w/d_{l})$$
(5.3)

where *n*, *p*, *r*, *s* and *t* are integers, the complex numbers  $a_{i}, b_{j}, c_{k}, d_{l}$  are unimodular in the limit  $N \rightarrow \infty$  and, by convention, f(w) still means  $f(w, x^{5})$ .

In (5.3) we have made the dependence of V(w) on the integers p and r explicit because these will label the bands of eigenvalues. From (3.17) and (3.18) we obtain the relations

$$2p + 2r + s + t = N$$
  $t = 2n.$  (5.4)

There is in fact another constraint on these integers. If we substitute (5.3) into the right-hand side of (3.16*a*) with  $w = ax^{-3}$ , we find that it vanishes for *n* choices of *a*. The left-hand side, however, is known to vanish if and only if  $a = a_i$  with i = 1, 2, ..., p or  $a = c_k$  with k = 1, 2, ..., s. Hence

$$n = p + s. \tag{5.5}$$

Since other choices of w in the above procedure give no further relations, we conclude that

$$n = \frac{1}{3}(N - p - 2r) \qquad p + 2r = N \pmod{3}$$
  

$$s = \frac{1}{3}(N - 4p - 2r) \qquad t = \frac{2}{3}(N - p - 2r).$$
(5.6)

Since p = O(1) and r = O(1) as  $N \to \infty$  for the largest eigenvalues, the requirement  $4p + 2r \le N$  for s to be non-negative is automatically satisfied.

To solve the transfer matrix equation (3.16) in the limit  $N \to \infty$ , i.e. to eliminate  $c_1, c_2, \ldots, c_s$  and  $d_1, d_2, \ldots, d_b$  we can now proceed as for regime I. Use (5.3) and (3.16c) to define  $T_{p,r}(w)$  and temporarily regard  $a_1, \ldots, a_p$  and  $b_1, \ldots, b_r$  as known. This function then factors into a known singular part and an unknown part whose logarithm is Laurent expansible in the annulus  $x^{1/2} < |w| < x^{-2}$ . Likewise,  $T_{p,r}(w)$  can be factored in the annulus  $x^3 < |w| < x^{1/2}$  but with a different unknown part. The coefficients of these expansions can then be obtained by equating coefficients on either side of (3.16a), retaining the different dominant terms in the two annuli  $x^{1/2} < |w| < x^{-1/2}$  and  $x^{-1} < |w| < x^{-3/2}$ . For N large, and (p, r) = (0, 0) = 0, this gives

$$T_0(w) = \tau \psi^N(w) \qquad x^{1/2} < |w| < x^{-2} \tag{5.7a}$$

where  $\tau$  is a cube root of unity, and for  $(p, r) \neq 0$ 

$$T_{p,r}(w) = \psi^{N}(w) \prod_{i=1}^{p} \psi(a_{i}w^{-1}) \prod_{j=1}^{r} \bar{\psi}(b_{j}w^{-1}) \qquad x^{1/2} < |w| < x^{-2}$$
(5.7b)

where

$$\psi(w) = -w^{1/3} \frac{f(xw^{-1}, x^3)}{f(xw, x^3)} \qquad \tilde{\psi}(w) = \psi(x^{3/2}w^{-1}) = w^{2/3} \frac{f(x^{1/2}w^{-1}, x^3)}{f(x^{1/2}w, x^3)}.$$
 (5.8)

The solution in the other half-period annulus is given by the relation

$$T_{p,r}(w) = T_{p,r}(xw^{-1}) \qquad x^3 < |w| < x^{1/2}.$$
(5.9)

If we set  $w = a_i x^2$  or  $b_j x^{1/2}$  in the transfer matrix equation (3.16*a*) the left-hand side vanishes and

$$1 + T_{p,r}(a_i) = 0 \qquad 1 + T_{p,r}(b_j x^{3/2}) = 0.$$
(5.10)

The  $a_i$  and  $b_j$  are therefore solutions of the equations

$$\psi^{N}(a_{i}) = -\prod_{k=1}^{p} \psi(a_{i}/a_{k}) \prod_{l=1}^{r} \bar{\psi}(a_{i}/b_{l}) \qquad i = 1, 2, \dots, p$$
  
$$\bar{\psi}^{N}(b_{j}) = -\prod_{k=1}^{p} \bar{\psi}(b_{j}/a_{k}) \prod_{l=1}^{r} \psi(b_{j}/b_{l}) \qquad j = 1, 2, \dots, r.$$
(5.11)

Again, since  $|\psi(w)| = |\bar{\psi}(w)| = 1$  when |w| = 1, these equations are consistent with the requirement that the  $a_i$  and  $b_i$  be unimodular.

In the physical regime  $1 \le w \le x^{-1}$ , and for large N, the largest eigenvalue of the transfer matrix V(w) is given by (5.7a) with  $\tau = 1$ . From (2.6) and (3.4), the partition function per site is

$$\kappa(w) = -\omega_4(w)\omega_5(w)\psi(w)/\omega_1(w)$$
(5.12)

where  $\omega_1(w)$ ,  $\omega_4(w)$  and  $\omega_5(w)$  are given by (3.14). Again we see that this agrees with the result (Baxter 1980a) previously obtained by the matrix inversion trick.

## 5.2. Interfacial tension

For (p, r) = 0 ( $N = 0 \mod 3$ ), we see that (5.7a) gives a triplet of largest eigenvalues. But this degeneracy cannot occur in the physical regime  $1 < w < x^{-1}$ , for finite N, by the Perron-Frobenius theorem. The triplet of eigenvalues is therefore asymptotically degenerate as  $N \rightarrow \infty$ . In the limit of large N, we in fact expect (Fisher 1969) that

$$V_{0;\tau}(w)/V_{0;1}(w) = \tau [1 - O(e^{-N\beta\sigma})] \qquad \tau \neq 1$$
(5.13)

where we have labelled the triplet of largest eigenvalues of V(w), in the obvious way, by the choice of the cube root  $\tau$  in (5.7*a*). The parameter  $\beta = 1/k_BT$  is the inverse temperature and  $\sigma$  is the interfacial tension.

To calculate  $\sigma$ , we repeat the above calculation of  $T_0(w)$ , keeping both terms on the right-hand side of (3.16*a*) and treating the smaller term as a correction. For  $1 < |w| < x^{-1}$  this gives

$$T_{\mathbf{0};\tau}(w) = \tau \psi^{N}(w) M_{\tau}(w)$$
(5.14*a*)

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where the correction term  $M_{\tau}(w)$  is given by

$$\ln M_{\tau}(w) = \frac{1}{2\pi i} \oint_{|w'|=1} \frac{dw'}{w'} \{ J(xw/w') \ln[1 + T_{0;\tau}(x^3w')] + J(w/w') \ln[1 + T_{0;\tau}^{-1}(x^2w')] \}$$
(5.14b)

and

$$J(w) = w\psi'(w)/\psi(w) \tag{5.15}$$

with  $\psi'(w)$  the derivative of  $\psi(w)$ . The integral equation (5.14) is exact, even for finite N.

From (5.13), the interfacial tension is now given by

$$-\beta\sigma = \lim_{N \to \infty} N^{-1} \ln \ln[T_{0;\tau}(w)/T_{0;1}(w)]$$
$$= \lim_{N \to \infty} N^{-1} \ln \ln[M_{\tau}(w)/M_{1}(w)]$$
(5.16)

with  $\tau^3 = 1$  and  $\tau \neq 1$ . For w' in the annulus  $x^{1/2} < |w'| < x^{-1/2}$  and N large, however, we find from (5.2) and (5.7a) that

$$\ln[1+T_{0;\tau}(x^{3}w')] \sim \tau \psi^{N}(xw') + \tau \psi^{N}(x/w') \qquad \ln[1+T_{0;\tau}^{-1}(x^{2}w')] \sim \tau \psi^{N}(xw').$$
(5.17)

Since  $N = 0 \pmod{3}$ ,  $\psi^N(w)$  is analytic in the annulus  $x^2 < |w| < x^{-1}$ . For large N, we can therefore put (5.17) into (5.14b) and integrate by steepest descents. Considered as a function of a real variable,  $\psi(w)$  has a single minimum at  $w = w_s$  with  $-x < w_s < -x^{3/2}$ . In the complex plane this corresponds to a saddle point of  $|\psi(w)|$ . For each term coming from (5.17) we find that the contour |w'| = 1 in (5.14b) can be deformed, without crossing the poles of J(w) at w = x and  $x^{-1}$ , to an equivalent contour through the saddle point  $w = w_s$ . Using (5.16), we finally obtain

$$-\beta\sigma = \ln\psi(w_s). \tag{5.18}$$

The same result can also be obtained by considering the limit of a large  $P \times N$  lattice, under the constraints  $P = 0 \pmod{3}$ , N = 1 or 2 (mod 3). These constraints introduce a mismatched vertical seam into the domain structure of the model. The interfacial tension is then related to the excess free energy above the bulk free energy for such a system. Let us consider the case  $N = 1 \pmod{3}$ . If  $\kappa(w)$  is the partition function per site for the bulk, as given by (2.6), then the interfacial tension  $\sigma$  is given by

$$-\beta\sigma = \lim_{P \to \infty} \lim_{N \to \infty} P^{-1} \ln \operatorname{Tr}[V^{P}(w) / \kappa^{PN}(w)].$$
(5.19)

If  $N = 1 \pmod{3}$ , (5.7b) and (5.11) give a band of N complex largest eigenvalues with p = 1 and r = 0. If we now make the usual assumption that in the limit  $N \to \infty$  the solutions  $a_1$  of (5.11) form a continuous distribution on the circle  $|a_1| = 1$  with density  $\rho(a_1)$ , we find that for large P

$$\lim_{N \to \infty} \operatorname{Tr}[\boldsymbol{T}(w)/T_{0;1}(w)]^{P} \sim \frac{1}{2\pi \mathrm{i}} \oint_{|a_{1}|=1} \frac{\mathrm{d}a_{1}}{a_{1}} \rho(a_{1}) \psi^{P}(a_{1}w^{-1}).$$
(5.20)

Again the lower bands of eigenvalues with  $p + r \ge 2$  should not contribute in the limit  $P \rightarrow \infty$ . As before, the integral can be evaluated by steepest descents, provided  $\rho(a_1)$  is analytic in the annulus  $x^{3/2} < |a_1| \le 1$  containing the saddle point  $a_1 = w_s w$ . Doing this we again obtain the interfacial tension as given by (5.18).

In the limit  $x \rightarrow 1-$ , i.e. at criticality, the interfacial tension vanishes. In the original parametrisation we find

$$\beta \sigma \sim 2\sqrt{3}(q^2)^{5/6} \qquad q^2 \to 0+.$$
 (5.21)

Hence the interfacial tension exponent is

$$\mu = 5/6.$$
 (5.22)

#### 5.3. Correlation length

We now turn to the calculation of the correlation length for  $1 \le w \le x^{-1}$ . If N = 3L, recall that p = r = 0 gives a triplet of largest eigenvalues. The next-largest eigenvalues are given by p = r = 1. In this case (5.7b) and (5.11) give a band of 6L(L-1) complex eigenvalues. Noting that  $|\psi(w)| \le 1$  for  $x^{3/2} \le |w| \le 1$ , we see that the gap between the largest and next-largest eigenvalues is

$$V_{1,1}(w)/V_{0,1}(w) = T_{1,1}(w)/T_{0,1}(w) = \psi(a_1w^{-1})\bar{\psi}(b_1w^{-1}).$$
(5.23)

We now repeat the arguments outlined for calculating the correlations in regime I. We find that the asymptotic behaviour of the correlation between sites separated by l rows, for l large, is

$$\langle \sigma_0 \sigma_l \rangle - \langle \sigma_0 \rangle \langle \sigma_l \rangle \sim \left( \frac{1}{6\pi i} \right)^2 \oint_{|a_1|=1} \frac{da_1}{a_1} \oint_{|b_1|=1} \frac{db_1}{b_1} \rho(a_1, b_1) \psi^l(a_1 w^{-1}) \bar{\psi}^l(b_1 w^{-1}).$$
 (5.24)

Here the contours are closed loops formed by three circuits about the origin on the Riemann surface of three sheets on which the function  $a \mapsto a^{1/3}$  is analytic. Except for poles on each sheet corresponding to  $w = x^{-1}, x^2$ , etc,  $\psi(w)$  is also analytic on this Riemann surface (its values on any two sheets differ only by a complex cube root of unity). For large *l*, it is therefore possible to evaluate the integral (5.24) by steepest descents.

As before, let  $w = w_s$  be the saddle point given by  $\psi'(w_s) = 0$  with  $-x < w_s < -x^{3/2}$ . Let us also assume that the density  $\rho(a_1, b_1)$  is analytic on the contours and can be analytically continued to the saddle points on each sheet corresponding to  $a_1 = w_s w$  and  $b_1 = x^{3/2} w/w_s$ . If the contours in (5.24) are then deformed to equivalent contours passing through these saddle points, we find that for large l

$$\langle \sigma_0 \sigma_l \rangle - \langle \sigma_0 \rangle \langle \sigma_l \rangle \sim e^{-l\xi^{-1}} [A + B \cos(\frac{2}{3}\pi l + \delta)]$$
(5.25)

where the correlation length  $\xi$  is given by

$$-\xi^{-1} = 2 \ln \psi(w_s). \tag{5.26}$$

Combining (5.18) and (5:26) we obtain the exact and intriguing relation (a corresponding relation exists for the eight-vertex model: Baxter (1981b), equation (10.10.14))

$$\beta \sigma \xi = \frac{1}{2}.\tag{5.27}$$

It follows that the correlation length diverges as  $x \rightarrow 1-$ , i.e. at criticality. In the original

parametrisation we also find that near criticality

$$\xi \sim \frac{1}{4\sqrt{3}} (q^2)^{-5/6} \qquad q^2 \to 0+.$$
 (5.28)

Hence the correlation exponent is

$$\nu' = 5/6.$$
 (5.29)

## References

Baxter R J 1972 Ann. Phys., NY 70 193-228

- ----- 1973 J. Stat. Phys. 8 25-55

----- 1981a J. Stat. Phys. in press

Fisher M E 1969 J. Phys. Soc. Japan, Suppl. 26 87-8

Johnson J D, Krinsky S and McCoy B M 1973 Phys. Rev. A 8 2526-47

Lieb E H and Wu F Y 1972 Two-dimensional Ferroelectric Models in Phase Transitions and Critical Phenomena vol 1, ed C Domb and M S Green (New York: Academic) pp 331-490

Shankar R 1981 Yale University, Physics Department Preprint YTP 81-21