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1989 J. Phys. A: Math. Gen. 22 1141

(http://iopscience.iop.org/0305-4470/22/8/027)

J. Phys. A: Math. Gen. 22 (1989) 1141-1165. Printed in the UK

Surface free energy of the critical six-vertex model with free boundaries

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Received 5 July 1988

Abstract. The Bethe ansatz equations are derived for the six-vertex model with general boundary weights on a lattice in a diagonal orientation. These are solved in the thermodynamic limit. Finite-size corrections to the free energy (for a restricted class of boundary weights, including those corresponding to a Potts model with free boundaries) are calculated in the critical region.

The first-order term gives the surface free energy of the model. The second-order term is found to be $-\pi kT\tan(\pi v/2\mu)c/48N'^2$ where $c=[1-6\mu^2/(\pi^2-\pi\mu)]$ is the conformal anomaly. This can be compared to $-\pi kT\sin(\pi v/\mu)c/6N'^2$ for a calculation on the lattice in the standard orientation and with periodic boundary conditions. This difference can be explained geometrically using conformal invariance.

1. Introduction

The development of a procedure to calculate finite-size corrections to the free energy of a lattice spin system and the related ground-state energy of a quantum spin chain has recently received considerable attention. The impetus for this work has been the connection between these corrections and the hypothesis of conformal invariance.

De Vega and Woynarovich (1985) have given a method for calculating the leading finite-size corrections for models soluble by the Bethe ansatz in the non-critical region. In particular they calculated the corrections to the ground state of the XXZ chain and the six-vertex model with periodic boundary conditions in this region ($\Delta<-1$).

The extension to the critical region ($|\Delta|<1$) was explored by Hamer (1985, 1986), and Avdeev and Dörfel (1986) in the context of the XXZ chain. Woynarovich and Eckle (1987) have provided an elegant method for the critical region: this technique has been applied by Hamer *et al* (1987) to the Potts and Ashkin-Teller quantum spin chains with both periodic and free boundaries and by de Vega and Karowski (1987) to the six-vertex model with periodic boundary conditions†.

Here we consider the six-vertex model on the square lattice turned through 45°, with free boundary conditions. In fact, we first allow the boundary weights to be arbitrary. This means that our model includes the regular square lattice Potts model with free boundaries (Baxter *et al* 1976).

† Karowski (1988) has extended this technique to calculate the scaling dimensions of models solvable by the Bethe ansatz and has considered the six-vertex and Potts models with periodic boundary conditions.

0305-4470/89/081141+25\$02.50

The model is explained and the Bethe ansatz equations are set up in a manner similar to Alcaraz *et al* (1987) in § 2. These are shown to give the known answer to the bulk free energy (Baxter 1982). The finite-size corrections (for a lattice of infinite height but finite width) are calculated in § 3. We use the method explained by Hamer *et al* (1987). The surface free energy and conformal anomaly term are given in equation (3.15). In the light of conformal invariance we discuss the results in § 4. A summary of this work is contained in § 5.

2. Bethe ansatz six-vertex model

Let us consider a six-vertex model on a rotated $M' \times N'$ lattice (where $M' \gg N' \gg 1$) as in figure 1. We place arrows on edges subject to the rule that at each site there be two arrows in and two out. There are then six internal configurations as in figure 2, with weights

$$\omega_1, \ldots, \omega_6 \equiv 1, 1, b, b, c, c' \tag{2.1}$$

and four external configurations with weights

$$\omega_7, \ldots, \omega_{10} \equiv 1, d, e, 1 \tag{2.2}$$

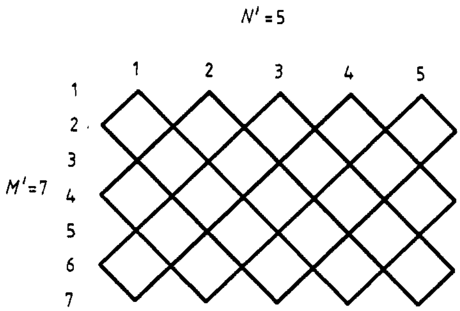

Figure 1. A 7×5 lattice of the rotated orientation.

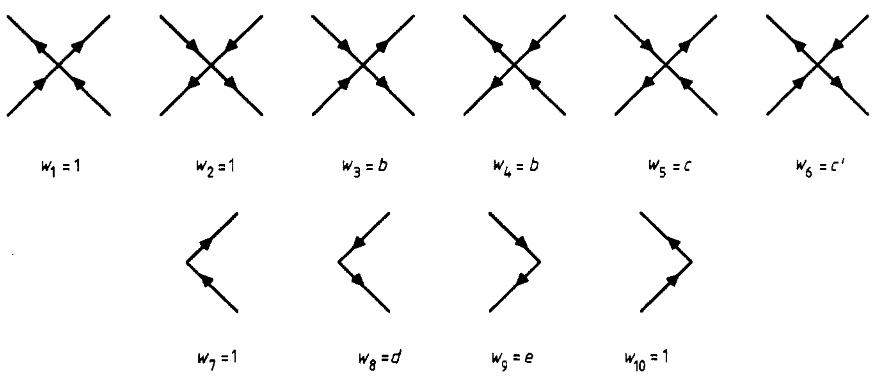

Figure 2. The six internal and four external weights of the six-vertex model on a rotated lattice.

where we have normalised the weights so that a configuration of all arrows up has total weight 1. The partition function Z is given by

$$Z = \sum_{\text{configurations}} \prod_{\text{vertices}} (\text{weights}). \tag{2.3}$$

There naturally exist two types of rows of vertices and two types of rows of edges as in figure 3. This leads us to define two transfer matrices $\mathbf{T}_1$ and $\mathbf{T}_2$. $\mathbf{T}_1(\mathbf{T}_2)$ is the matrix of all the weights of configurations of a type 1 (2) row of vertices. The transfer matrices $\mathbf{T}_1(\mathbf{T}_2)$ can be viewed as adding a row of edges of types 2 (1) to the lattice. The partition function can be written as

$$Z = \mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2)^{M'/2}. \tag{2.4}$$

(We choose periodic boundary conditions on the first and last rows since it is the free boundary columns that dominate in finite-size corrections as $M' \gg N'$. We choose M' to be even.)

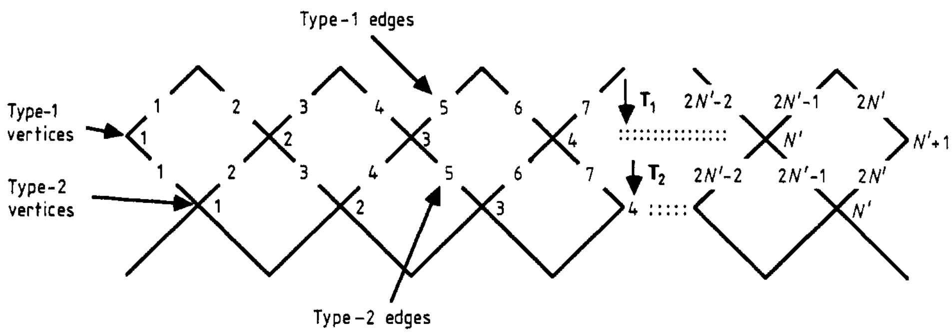

Figure 3. Examples of the two different types of rows of vertices and edges that occur in this model. A $\mathbf{T}_1$ ($\mathbf{T}_2$) transfer matrix acts on a type-1 (2) row of edges to add a type-2 (1) row of edges. In doing so it creates a type-1 (2) row of vertices.

Let us now examine any particular configuration of the arrows on the lattice. We notice that, if the configuration of one row contains a number n of down arrows on the $2N' = N$ edges, then each row has n down arrows. This observation provides us with a good 'quantum' number n of the matrices $\mathbf{T}_1$ and $\mathbf{T}_2$ since they split into $N+1$ diagonal blocks characterised by n.

We identify a state of a type 1 (or 2) row of edges by defining the positions of the down arrows of the configuration

$$1 \leqslant x_1 < x_2 < \ldots < x_n \leqslant N. \tag{2.5}$$

Let $\boldsymbol{x} = \{x_1, \ldots, x_n\}$ and $\boldsymbol{G}(\boldsymbol{x})$ and $\boldsymbol{F}(\boldsymbol{x})$ be the elements of vectors, defined on a type-1 and type-2 row of edges, respectively, having the property

$$\Lambda \boldsymbol{F}(\boldsymbol{x}) = \sum_{\boldsymbol{y}} \mathbf{T}_1(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{G}(\boldsymbol{y}) \tag{2.6a}$$

$$\Lambda \boldsymbol{G}(\boldsymbol{x}) = \sum_{\boldsymbol{y}} \mathbf{T}_2(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{F}(\boldsymbol{y}). \tag{2.6b}$$

We deduce

$$\Lambda^2 \boldsymbol{G} = \mathbf{T}_2\mathbf{T}_1\boldsymbol{G} \tag{2.7a}$$

and

$$\Lambda^2 \boldsymbol{F} = \mathbf{T}_1 \mathbf{T}_2 \boldsymbol{F} \tag{2.7b}$$

so $\boldsymbol{G}(\boldsymbol{F})$ is the eigenvector of the two-row transfer matrix $\mathbf{T}_2\mathbf{T}_1$ ($\mathbf{T}_1\mathbf{T}_2$), and Λ^2 is the eigenvalue. It follows that the partition function is asymptotically

$$Z \sim \Lambda_{\max}^{M'} \tag{2.8}$$

where $\Lambda_{\max}^2$ is the largest eigenvalue of $\mathbf{T}_1\mathbf{T}_2$.

We can consider the eigenvalue problem (2.7) for a particular n. We start by considering equations (2.6) for $n = 0$, then $n = 1$, moving onto $n = 2$ and then generalising to arbitrary n as is the usual procedure (Baxter 1982, Alcaraz *et al* 1987). We follow a notation similar to Alcaraz *et al* (1987).

2.1. The case $n = 0$ (no down arrows)

This case corresponds to a state where all the arrows in a row are up. We have deliberately chosen the weights so that

$$\Lambda F = G \tag{2.9a}$$

and

$$\Lambda G = F. \tag{2.9b}$$

Hence

$$\Lambda = \pm 1 \qquad \text{so } F = \pm G. \tag{2.10}$$

2.2. The case $n = 1$ (one down arrow)

The transfer matrix equations (2.6) become

$$\Lambda \boldsymbol{F}(x) = \sum_{x'} \mathbf{T}_1(x, x') \boldsymbol{G}(x') \tag{2.11a}$$

$$\Lambda \boldsymbol{G}(x) = \sum_{x'} \mathbf{T}_2(x, x') \boldsymbol{F}(x') \tag{2.11b}$$

where $\boldsymbol{F}(x)$ (respectively $\boldsymbol{G}(x)$) is the element of $\boldsymbol{F}$ (respectively ($\boldsymbol{G}$)) for one down arrow in the x position along the row.

Explicitly

$$\Lambda F(x) = cG(x) + bG(x+1) \qquad x = 2, \ldots, N-2 \tag{2.12a}$$

$$\Lambda F(x) = bG(x-1) + c'G(x) \qquad x = 3, \ldots, N-1 \tag{2.12b}$$

$$\Lambda G(x) = cF(x) + bF(x+1) \qquad x = 1, \ldots, N-1 \tag{2.12c}$$

$$\Lambda G(x) = bF(x-1) + c'F(x) \qquad x = 2, \ldots, N \tag{2.12d}$$

with the boundary conditions

$$\Lambda F(1) = dG(1) \tag{2.13a}$$

$$\Lambda F(N) = eG(N) \tag{2.13b}$$

where N is the number of edges in a row of the lattice.

We now choose an ansatz for $F(x)$ and $G(x)$. We notice that there are different equations for odd and even x. First look for a solution

$$F(x)=f(x,k) \tag{2.14a}$$

$$G(x)=g(x,k) \tag{2.14b}$$

$$\Lambda=\lambda(k) \tag{2.14c}$$

where

$$f(x,k)=A_e(k)\,\mathrm{e}^{\mathrm{i}kx} \qquad x \text{ even} \tag{2.15a}$$

$$f(x,k)=A_0(k)\,\mathrm{e}^{\mathrm{i}kx} \qquad x \text{ odd} \tag{2.15b}$$

$$g(x,k)=B_e(k)\,\mathrm{e}^{\mathrm{i}kx} \qquad x \text{ even} \tag{2.15c}$$

$$g(x,k)=B_0(k)\,\mathrm{e}^{\mathrm{i}kx} \qquad x \text{ odd.} \tag{2.15d}$$

Substituting this ansatz into (2.12) we obtain

$$\lambda(k)A_e(k)=cB_e(k)+bB_0(k)\,\mathrm{e}^{\mathrm{i}k} \tag{2.16a}$$

$$\lambda(k)A_0(k)=bB_e(k)\,\mathrm{e}^{-\mathrm{i}k}+c'B_0(k) \tag{2.16b}$$

$$\lambda(k)B_0(k)=cA_0(k)+bA_e(k)\,\mathrm{e}^{\mathrm{i}k} \tag{2.16c}$$

$$\lambda(k)B_e(k)=bA_0(k)\,\mathrm{e}^{-\mathrm{i}k}+c'A_e(k). \tag{2.16d}$$

We can now eliminate $B_0(k)$ and $B_e(k)$ to find

$$(\lambda^2(k)-cc'-b\,\mathrm{e}^{2\mathrm{i}k})A_e(k)=2bc\cos(k)A_0(k) \tag{2.17a}$$

$$(\lambda^2(k)-cc'-b\,\mathrm{e}^{-2\mathrm{i}k})A_0(k)=2bc'\cos(k)A_e(k) \tag{2.17b}$$

and finally eliminate the ratio $A_0(k)/A_e(k)$ to obtain

$$(\lambda^2(k)-cc'-b\,\mathrm{e}^{2\mathrm{i}k})(\lambda^2(k)-cc'-b\,\mathrm{e}^{-2\mathrm{i}k})=4b^2cc'\cos^2 k. \tag{2.18}$$

We notice that (2.18) is invariant under the transformation $k\to -k$. This implies that the trial solution (2.14) under the transformation $k\to -k$ also gives the same value of Λ^2.

We notice also that the ratio $A_0(k)/A_e(k)$ plays an important role in these equations so we define

$$r(k)=\frac{f(x+1,k)}{f(x,k)} \qquad x \text{ odd}$$
$$=\frac{A_e(k)\,\mathrm{e}^{\mathrm{i}k}}{A_0(k)} \tag{2.19}$$

and

$$t(k)=\frac{f(x+1,k)}{f(x,k)} \qquad x \text{ even}$$
$$=\frac{A_0(k)\,\mathrm{e}^{\mathrm{i}k}}{A_e(k)}. \tag{2.20}$$

Now using (2.19) and (2.20) we write (2.17) as

$$\left(\frac{\lambda^2(k) - cc' - b^2 \,\mathrm{e}^{2\mathrm{i}k}}{2b \cos k}\right) = ct(k)\,\mathrm{e}^{-\mathrm{i}k} \tag{2.21a}$$

$$\left(\frac{\lambda^2(k) - cc' - b^2 \,\mathrm{e}^{-2\mathrm{i}k}}{2b \cos k}\right) = c'r(k)\,\mathrm{e}^{-\mathrm{i}k}. \tag{2.21b}$$

But both these equations are necessarily invariant under the transformation $k \to -k$ so

$$c'r(k)\,\mathrm{e}^{-\mathrm{i}k} = ct(-k)\,\mathrm{e}^{\mathrm{i}k} \tag{2.22a}$$

$$ct(k)\,\mathrm{e}^{-\mathrm{i}k} = c'r(-k)\,\mathrm{e}^{\mathrm{i}k}. \tag{2.22b}$$

From the definitions (2.19) and (2.20) we know

$$r(k)t(k) = \mathrm{e}^{2\mathrm{i}k} \tag{2.23}$$

so (2.22) gives

$$t(k)t(-k) = [r(k)r(-k)]^{-1} = c'/c. \tag{2.24}$$

Using (2.21) and (2.23) we can show that

$$t(k) = \frac{b + c'r(k)}{c + br(k)}. \tag{2.25}$$

Also, using (2.21) and (2.23) we have

$$\lambda^2(k) = cc' + bc\left(t(k) + \frac{1}{r(k)}\right) + b^2 r(k)t(k). \tag{2.26}$$

Our trial solution (2.14) has not only succeeded and given us $\lambda(k)$ as (2.26) but led to a new solution via a transformation $k \to -k$ on (2.14) because $\lambda(k) = \lambda(-k)$. Hence any linear combination of these two solutions is a solution of (2.12). We try a linear combination of these solutions as our ansatz, attempting to choose coefficients to satisfy the boundary conditions (2.13):

$$F(x) = A(k)f(x, k) - A(-k)f(x, -k) \tag{2.27a}$$

$$G(x) = A(k)g(x, k) - A(-k)g(x, -k). \tag{2.27b}$$

This ansatz now automatically satisfies (2.12). We want to choose k and $A(-k)/A(k)$ to satisfy (2.13).

We extend the definitions of our ansatz $F(x)$ to $x = 0$ and $x = N+1$, correspondingly extending (2.12):

$$\Lambda F(0) = cG(0) + bG(1) \tag{2.28a}$$

$$\Lambda F(1) = bG(0) + c'G(1) \tag{2.28b}$$

$$\Lambda F(N) = cG(N) + bG(N+1) \tag{2.28c}$$

$$\Lambda F(N+1) = bG(N) + c'G(N+1). \tag{2.28d}$$

We then combine (2.28) with (2.13), eliminating $G(0)$, $G(1)$, $G(N)$ and $G(N+1)$ to give

$$F(0) + \delta F(1) = 0 \tag{2.29a}$$

and

$$F(N+1)+\delta' F(N)=0 \tag{2.29b}$$

where

$$\delta=\frac{cc'}{bd}-\frac{b}{d}-\frac{c}{b} \tag{2.30a}$$

$$\delta'=\frac{cc'}{be}-\frac{b}{e}-\frac{c'}{b}. \tag{2.30b}$$

Equations (2.29) are equivalent to the original boundary conditions (2.13) in the sense that if they and (2.28) are satisfied then so is (2.13). We now substitute our ansatz into (2.29) to find

$$\alpha(k)A(k)-\alpha(-k)A(-k)=0 \tag{2.31a}$$

and

$$\beta(k)A(k)-\beta(-k)A(-k)=0 \tag{2.31b}$$

where

$$\alpha(k)=1+\delta t(k) \tag{2.32a}$$

$$\beta(k)=(t(k)+\delta')[r(k)t(k)]^{N/2}. \tag{2.32b}$$

We note that (2.13b) is satisfied if $A(k)$ satisfies the functional relation

$$A(k)=\beta(-k) \qquad \forall k \tag{2.33}$$

(which of course implies $A(-k)=\beta(k)$).

Then (2.31a) gives

$$\frac{\alpha(k)\beta(-k)}{\alpha(-k)\beta(k)}=1 \tag{2.34}$$

which is the Bethe ansatz equation for the $n=1$ case. This equation can now, in principle, be used to solve for k. Hence (2.33) and (2.34) completely specify our ansatz (2.27) (up to a multiplicative factor). The Bethe ansatz equation (2.34) is of the form

$$\eta(k)z^{2N}=1 \tag{2.35a}$$

where

$$z=\mathrm{e}^{-ik} \qquad \eta(k)=\left(\frac{1+\delta t(k)}{1+t(k)/\delta'}\right)\left(\frac{1+t(-k)/\delta'}{1+\delta t(-k)}\right). \tag{2.35b}$$

Hence we can find N distinct solutions for k (and also for $-k$) and so we have N eigenvalues $\lambda^2(k)$ for the $N\times N$ matrix $\mathbf{T}_1\mathbf{T}_2$. We therefore have in (2.34) a complete solution for the eigenvalue problem (2.7).

2.3. *The case $n=2$ (two down arrows)*

The transfer matrix equations (2.6) become

$$\Lambda F(x_1,x_2)=\sum_{(x_1',x_2')}\mathbf{T}_1(x_1,x_2;x_1',x_2')G(x_1',x_2') \tag{2.36a}$$

$$\Lambda G(x_1,x_2)=\sum_{(x_1',x_2')}\mathbf{T}_2(x_1,x_2;x_2',x_2')F(x_1',x_2') \tag{2.36b}$$

where $F(x_1, x_2)$ (respectively $G(x_1, x_2)$) is the element of $\boldsymbol{F}$ (respectively $(\boldsymbol{G})$) for two down arrows in the positions x_1 and x_2 with $x_1 < x_2$. These are explicitly

$$\Lambda F(x_1, x_2) = b^2 G(x_1+1, x_2+1) + bcG(x_1, x_2+1) + bcG(x_1+1, x_2) + c^2 G(x_1, x_2) \qquad \text{when } x_1 \text{ and } x_2 \text{ are even} \tag{2.37a}$$

$$\Lambda F(x_1, x_2) = b^2 G(x_1+1, x_2-1) + bcG(x_1, x_2-1) + bc'G(x_1+1, x_2) + cc'G(x_1, x_2) \qquad \text{when } x_1 \text{ is even and } x_2 \text{ is odd} \tag{2.37b}$$

$$\Lambda F(x_1, x_2) = b^2 G(x_1-1, x_2+1) + bc'G(x_1, x_2+1) + bcG(x_1-1, x_2) + cc'G(x_1, x_2) \qquad \text{when } x_1 \text{ is odd and } x_2 \text{ is even} \tag{2.37c}$$

$$\Lambda F(x_1, x_2) = b^2 G(x_1-1, x_2-1) + bc'G(x_1, x_2-1) + bc'G(x_1-1, x_2) + c'^2 G(x_1, x_2) \qquad \text{when } x_1 \text{ and } x_2 \text{ are odd} \tag{2.37d}$$

$$\Lambda G(x_1, x_2) = b^2 F(x_1-1, x_2-1) + bc'F(x_1, x_2-1) + bc'F(x_1-1, x_2) + c'^2 F(x_1, x_2) \qquad \text{when } x_1 \text{ and } x_2 \text{ are even} \tag{2.38a}$$

$$\Lambda G(x_1, x_2) = b^2 F(x_1-1, x_2+1) + bc'F(x_1, x_2+1) + bcF(x_1-1, x_2) + c'cF(x_1, x_2) \qquad \text{when } x_1 \text{ is even and } x_2 \text{ is odd} \tag{2.38b}$$

$$\Lambda G(x_1, x_2) = b^2 F(x_1+1, x_2-1) + bcF(x_1, x_2-1) + bc'F(x_1+1, x_2) + c'cF(x_1, x_2) \qquad \text{when } x_1 \text{ is odd and } x_2 \text{ is even} \tag{2.38c}$$

$$\Lambda G(x_1, x_2) = b^2 F(x_1+1, x_2+1) + bcF(x_1, x_2+1) + bcF(x_1+1, x_2) + c^2 F(x_1, x_2) \qquad \text{when } x_1 \text{ and } x_2 \text{ are odd} \tag{2.38d}$$

and on the boundaries we have

$$\Lambda F(1, x_1) = d[cG(1, x_2) + bG(1, x_2+1)] \qquad \text{when } x_2 \text{ is even} \tag{2.39a}$$

$$\Lambda F(1, x_2) = d[c'G(1, x_2) + bG(1, x_2-1)] \qquad \text{when } x_2 \text{ is odd} \tag{2.39b}$$

$$\Lambda F(x_1 N) = e[cG(x_1, N) + bG(x_1+1, N)] \qquad \text{when } x_1 \text{ is even} \tag{2.39c}$$

$$\Lambda F(x_1, N) = e[c'G(x_1, N) + bG(x_1-1, N)] \qquad \text{when } x_1 \text{ is odd.} \tag{2.39d}$$

We also have the meeting conditions:

$$\Lambda F(x_1, x_1+1) = G(x_1, x_1+1) \qquad \text{when } x_1 \text{ is even} \tag{2.40a}$$

and

$$\Lambda G(x_1, x_1+1) = F(x_1, x_1+1) \qquad \text{when } x_1 \text{ is odd.} \tag{2.40b}$$

Using (2.37) and (2.38), we can write (2.40) as

$$b^2 F(x_1+1, x_1) + bcF(x_1, x_2) + bc'F(x_1+1, x+1) + (cc'-1)F(x_1, x+1) = 0 \qquad \text{when } x_1 \text{ is odd} \tag{2.41a}$$

$$b^2 G(x_1+1, x_1) + bcG(x_1, x_2) + bc'G(x_1+1, x_1+1) + (cc'-1)G(x_1, x_1+1) = 0 \qquad \text{when } x \text{ is even.} \tag{2.41b}$$

We now choose our ansatz guided by the $n=1$ case and (2.20) of Alcaraz *et al* (1987) as

$$F(x_1, x_2) = \sum_P \varepsilon_P A(k_1, k_2) f(x_1, k_1) f(x_2, k_2) \tag{2.42a}$$

$$G(x_1, x_2) = \sum_P \varepsilon_P A(k_1, k_2) g(x_1, k_1) g(x_2, k_2) \tag{2.42b}$$

where $f(x, k)$ and $g(x, k)$ are the 'single-particle wavefunctions' defined in (2.15), the sum extends over all permutations and negations of the k and ε_P changes sign on each 'mutation'. Thus there are $2! \times 2^2 = 8$ terms in each P sum in (2.42).

Now (2.37) and (2.38) are automatically satisfied by each of the eight terms of the sum, provided only that

$$\Lambda = \lambda(k_1)\lambda(k_2). \tag{2.43}$$

As with the $n=1$ case, we can simplify the boundary conditions (2.39) by extending (2.42) to $x_1 = 0$, $x_2 = 0$, $x_1 = N+1$ and $x_2 = N+1$. Using (2.37) and (2.38), the boundary conditions (2.39) simplify to

$$F(0, x_2) + \delta F(1, x_2) = 0 \qquad \forall x_2 \tag{2.44a}$$

$$F(x_1, N+1) + \delta' F(x_1, N) = 0 \qquad \forall x_1. \tag{2.44b}$$

Using our ansatz in (2.44) we have

$$\alpha(k_1) A(k_1, k_2) - \alpha(-k_1) A(-k_1, k_2) = 0 \tag{2.45a}$$

$$\beta(k_2) A(k_1, k_2) - \beta(-k_2) A(k_1, -k_2) = 0. \tag{2.45b}$$

As well as (2.45a) and (2.45b) there are three other equations for each, obtained from these either by a negation of k_2 (2.45a) or k_1 (2.45b), or a permutation of k_1 and k_2, or both. We thus have eight equations.

We now substitute our ansatz into the meeting condition (2.40a) to obtain

$$s(k_1, k_2) A(k_1, k_2) - s(k_2, k_1) A(k_2, k_1) = 0 \tag{2.46}$$

where

$$s(k_1, k_2) = 1 + \frac{b}{c} r_1 + \frac{cc' - 1}{bc} r_2 + \frac{c'}{c} r_1 r_2. \tag{2.47}$$

Again, three other equations can be found by negating k_1, k_2 or both. Equation (2.40b) is now automatically satisfied.

By using (2.46), (2.45b) and (2.45a) to successively express $A(k_1, k_2)$ in terms of $A(k_2, k_1)$, $A(k_2, -k_1)$, $A(-k_1, k_2)$ and $A(k_1, k_2)$, we obtain the compatibility condition

$$\frac{\alpha(-k_1)\beta(k_1)}{\alpha(k_1)\beta(-k_1)} = \frac{B(-k_1, k_2)}{B(k_1, k_2)} \tag{2.48}$$

where

$$B(k, k') = s(k, k') s(k', -k). \tag{2.49}$$

As there are eight functions that can be obtained from $A(k_1, k_2)$ by mutations, we have eight compatibility conditions. However, because $s(k, k')$ has the property

$$r(-k_1) s(-k_1, -k_2) = r(k_2) s(k_2, k_1) \tag{2.50}$$

and both sides of (2.48) are of the form

$$\frac{y(k_1)}{y(-k_1)} \tag{2.51}$$

(2.48) is invariant under negations, so we only obtain one new equation through permutation, namely

$$\frac{\alpha(-k_2)\beta(k_2)}{\alpha(k_2)\beta(-k_2)}=\frac{B(-k_2, k_1)}{B(k_2, k_1)}. \tag{2.52}$$

Therefore we have two equations for the two unknowns k_1 and k_2 so, in principle, we can solve for them. Then $A(k_1, k_2)$ is given, for all k_1, k_2, by

$$A(k_1, k_2)=\frac{\beta(-k_1)\beta(-k_2)B(-k_1, k_2)}{r(k_2)} \tag{2.53}$$

and all the requirements (2.45) and (2.46) are fulfilled. Equations (2.48) and (2.52) are the Bethe ansatz equations for this $n=2$ case.

2.4. General n

The $n=2$ case results can be generalised to arbitrary values of n.

The ansatz becomes

$$F(x_1, \ldots, x_n)=\sum_P \varepsilon_P A(k_1, \ldots, k_n)f(x_1, k_1)\ldots f(x_n, k_n) \tag{2.54a}$$

and

$$G(x_1, \ldots, x_n)=\sum_P \varepsilon_P A(k_1, \ldots, k_n)g(x_1, k_1)\ldots g(x_n, k_n) \tag{2.54b}$$

where $f(x, k)$ and $g(x, k)$ are the single-particle wavefunctions, the sum extends over all negations and permutations of the k, and ε_P changes sign at each mutation.

Each term in (2.54) will automatically satisfy the 'free' equations of the general eigenvalue problem (2.6). The ansatz (2.54) therefore yields the eigenvalue

$$\Lambda=\lambda(k_1)\ldots\lambda(k_n). \tag{2.55}$$

The substitution of our ansatz into the boundary conditions will give

$$\alpha(k_1)A(k_1, \ldots, k_n)-\alpha(-k_1)A(-k_1, k_2, \ldots, k_n)=0 \tag{2.56a}$$

and

$$\beta(k_n)A(k_1, \ldots, k_n)-\beta(-k_n)A(k_1, \ldots, k_{n-1}, -k_n)=0. \tag{2.56b}$$

The 'meeting' conditions give

$$s(k_j, k_{j+1})A(\ldots, k_j, k_{j+1}, \ldots)-s(k_{j+1}, k_j)A(\ldots, k_{j+1}, k_j, \ldots)=0. \tag{2.57}$$

Again, other equations are found from these by appropriate negations and permutations. Importantly, the conditions (2.56b) and (2.57) are automatically satisfied by

$$A(k_1, \ldots, k_n)=\prod_{j=1}^{n}\beta(-k_j)\prod_{1\leqslant j<l\leqslant n}\frac{B(-k_j, k_l)}{r(k_l)}. \tag{2.58}$$

We then see that (2.56a) is satisfied, provided

$$\frac{\alpha(-k_j)\beta(k_j)}{\alpha(k_j)\beta(-k_j)}=\prod_{\substack{l=1\\ \neq j}}^{n}\frac{B(-k_j, k_l)}{B(k_j, k_l)} \qquad j=1, \ldots, n. \tag{2.59}$$

The n compatibility conditions are the Bethe ansatz equations for general n. They can, in principle, be used to solve for the n unknowns k_j. Then (2.58) will give the coefficients $A(k_1, \ldots, k_n)$. Again it is due to the special properties of the functions in these equations that we have n equations and not $2^n n!$ as one might expect from the number of functions $A(k_1 \ldots, k_n)$ produced by mutation.

2.5. *Special case (including Potts model)*

A significant feature of equations (2.59) is that the left-hand side simplifies if the condition

$$\delta\delta' = 1 \tag{2.60}$$

holds. The Bethe ansatz equations then become

$$\exp(\mathrm{i}2Nk_j) = \prod_{\substack{l=1\\ \neq j}}^{n} \frac{B(-k_j, k_l)}{B(k_j, k_l)} \qquad j = 1, \ldots, n. \tag{2.61}$$

Up until now we have considered the six-vertex model on a lattice of rotated orientation with general boundary weights. But Baxter *et al* (1976) derived an equivalence between the q-state Potts model on a square lattice $\mathscr{L}$ of standard orientation and a staggered six-vertex model on the medial lattice $\mathscr{L}'$. The partition function is

$$Z_{\text{Potts}} = \sum_S \exp\left(K \sum_{\langle i,j \rangle} \delta(S_i, S_j) + L \sum_{\langle j,k \rangle} \delta(S_j, S_k) \right) \tag{2.62}$$

where K and L are the interaction coefficients in the horizontal and vertical directions, the Potts spins $S_1, \ldots, S_{N'M'/2}$ each take on the values $1, \ldots, q$, the $\langle i, j \rangle$ sum is over all horizontal edges of $\mathscr{L}$ and the $\langle j, k \rangle$ sum is over all vertical edges. Furthermore, the condition

$$(\mathrm{e}^K - 1)(\mathrm{e}^L - 1) = q \tag{2.63}$$

for self-duality of the model is applied.

The first relevant feature of the equivalence established by Baxter *et al* (1976) is that the corresponding medial lattice $\mathscr{L}'$ is in the rotated orientation and of size $M' \times N'$ (see figure 7 of Baxter *et al* (1976)). Second, the internal weights of the six-vertex model, equivalent to this Potts model, are

$$\omega_1, \ldots, \omega_6 \equiv 1, 1, x, x, t^{-1} + xt, t + xt^{-1} \tag{2.64}$$

where

$$x = (\mathrm{e}^K - 1)q^{-1/2} = q^{1/2}/(\mathrm{e}^L - 1) \tag{2.65a}$$

and

$$t^2 + t^{-2} = q^{1/2}. \tag{2.65b}$$

Last, we take the boundary conditions on the Potts model to be 'free'. The external weights of the equivalent six-vertex model are

$$\omega_7, \ldots, \omega_{10} \equiv 1, t, t^{-1}, 1. \tag{2.66}$$

Now, making the correspondences

$$b = x \qquad c = t^{-1} + xt \qquad c' = t + xt^{-1} \qquad d = t \qquad e = t^{-1} \tag{2.67}$$

the six-vertex model equivalent to this self-dual q-state Potts model with free boundaries is a special case of our six-vertex model.

The partition functions are related via

$$Z_{\mathrm{Potts}} = q^{P/2} x^{-P} Z_{6\mathrm{V}} \tag{2.68}$$

where $Z_{6\mathrm{V}}$ is the partition function defined by (2.3) for our model and $P = M' \times N'$.

But now we notice

$$\delta = t^{-3} \qquad \delta' = t^3 \tag{2.69}$$

so that condition (2.60) is satisfied. Therefore the simplified Bethe ansatz equations (2.61) apply to the self-dual q-state Potts model with free boundary conditions.

In the next subsections we consider the Bethe ansatz equations in the form (2.61) and in the critical region of the model. Hence our calculations apply to the above Potts model for $q < 4$.

2.6. *Thermodynamic limit (critical region)*

We consider the 'general n' equations with the condition (2.60). We use a parametric substitution for the internal weights as follows:

$$a:b:c:c' \equiv 1 : \frac{\sin v}{\sin(\mu - v)} : \frac{\mathrm{e}^{\tau} \sin \mu}{\sin(\mu - v)} : \frac{\mathrm{e}^{-\tau} \sin \mu}{\sin(\mu - v)} \qquad 0 < \mu < \pi, |v| < \mu. \tag{2.70}$$

We can define the familiar $\Delta = -\cos \mu$ so $|\Delta| < 1$, which places the system in its critical region. Making the transformation

$$r(k) = \mathrm{e}^{\tau} \frac{\sin[(\mu - v)/2 + \mathrm{i}\alpha]}{\sin[(\mu - v)/2 - \mathrm{i}\alpha]} \tag{2.71}$$

and

$$t(k) = \mathrm{e}^{-\tau} \frac{\sin[(\mu + v)/2 + \mathrm{i}\alpha]}{\sin[(\mu + v)/2 - \mathrm{i}\alpha]} \tag{2.72}$$

we can show that

$$\frac{s(k_j, k_l)}{s(k_l, k_j)} = \frac{\sin[\mu - \mathrm{i}(\alpha_j - \alpha_l)]}{\sin[\mu + \mathrm{i}(\alpha_j + \alpha_l)]} \tag{2.73}$$

so the Bethe ansatz equations are from (2.59)

$$\left(\frac{\sin[(\mu - v)/2 + \mathrm{i}\alpha_j]\sin[(\mu + v)/2 + \mathrm{i}\alpha_j]}{\sin[(\mu - v)/2 - \mathrm{i}\alpha_j]\sin[(\mu + v)/2 - \mathrm{i}\alpha_j]}\right)^N = \prod_{\substack{l=1 \\ \neq j}}^{n} \left(\frac{\sin[\mu + \mathrm{i}(\alpha_j - \alpha_l)]\sin[\mu + \mathrm{i}(\alpha_j + \alpha_l)]}{\sin[\mu - \mathrm{i}(\alpha_j - \alpha_l)]\sin[\mu - \mathrm{i}(\alpha_j + \alpha_l)]}\right) \qquad j = 1, \ldots, n. \tag{2.74}$$

We notice that these expressions defining the roots α_j are independent of τ, d and e, so that these 'wavenumber' variables α_j depend only on the internal variables μ and v (i.e. only on the vertex weights b and the product cc').

We now follow the procedure in Baxter (1982), Gaudin (1983) and Hamer *et al* (1987). Defining

$$\phi(\alpha,\mu)=2\tan^{-1}(\cot\mu\tanh\alpha)$$
$$=\mathrm{i}\ln\left(\frac{\sinh(\mathrm{i}\mu+\alpha)}{\sinh(\mathrm{i}\mu-\alpha)}\right) \tag{2.75}$$

and taking the logarithm of (2.74) we have the Bethe ansatz equations as

$$N[\phi(\alpha_j,(\mu-v)/2)+\phi(\alpha_j,(\mu+v)/2)]=2\pi I_j+\sum_{\substack{l=1\\ \neq j}}^{n}[\phi(\alpha_j-\alpha_l,\mu)+\phi(\alpha_j+\alpha_l,\mu)] \tag{2.76}$$

where the I_j are integers.

The maximum eigenvalue for given n has

$$I_j=j \qquad j=1,\ldots,n \tag{2.77}$$

(Gaudin 1971, 1983). The value of n that produces the largest eigenvalue is $n=N/2$. We then must solve (2.76) for these conditions if we want the partition function for large N.

As in de Vega and Woynarovich (1985) we define

$$Z_N(\alpha)=\frac{1}{2\pi}\left[\phi\left(\alpha,\frac{\mu-v}{2}\right)+\phi\left(\alpha,\frac{\mu+v}{2}\right)\right]$$
$$+\frac{1}{2\pi N}[\phi(2\alpha,\mu)+\phi(\alpha,\mu)]-\frac{1}{2\pi N}\sum_{l=-n}^{n}\phi(\alpha-\alpha_l,\mu) \tag{2.78}$$

so that

$$Z_N(\alpha_j)=I_j/N \tag{2.79}$$

making the roots uniformly spread in the variable Z as pointed out by Hamer *et al* (1987).

We denote

$$\rho_N(\alpha)=\mathrm{d}Z_N(\alpha)/\mathrm{d}\alpha. \tag{2.80}$$

In taking the thermodynamic limit ($N\to\infty$) the roots α_j form a continuous distribution with density $N\rho_N(\alpha)$ and the sums become integrals. We conclude that

$$\rho_\infty(\alpha)=\frac{1}{2\pi}[\phi'(\alpha,(\mu-v)/2)+\phi'(\alpha,(\mu+v)/2)]-\int_{-\infty}^{\infty}\frac{\mathrm{d}\beta}{2\pi}\rho_\infty(\beta)\phi'(\alpha-\beta,\mu) \tag{2.81}$$

where

$$\int_{-\infty}^{\infty}\rho_\infty(\beta)\,\mathrm{d}\beta=1. \tag{2.82}$$

In appendix 1 we solve (2.81) by Fourier transforms to obtain

$$\rho_\infty(\alpha)=\frac{2\cos(\pi v/2\mu)\cosh(\pi\alpha/\mu)}{\mu[\cosh(2\pi\alpha/\mu)+\cos(\pi v/\mu)]}. \tag{2.83}$$

This is clearly different from the result for the Bethe ansatz equations of the six-vertex model on a lattice of standard orientation.

2.7. Free energy ($|\Delta| < 1$)

The free energy is given by

$$f = \frac{-kT}{N'M'} \ln Z \tag{2.84}$$

and so asymptotically can be given as

$$f = -kT \ln \Lambda_{\max}^{2/N}. \tag{2.85}$$

Now

$$\Lambda_{\max}^2 = \prod_{j=1}^{n} \psi(\alpha_j) \tag{2.86}$$

where

$$\psi(\alpha) = \frac{\sinh[\mathrm{i}(\mu+v)/2-\alpha]\sinh[\mathrm{i}(\mu+v)/2+\alpha]}{\sinh[\mathrm{i}(\mu-v)/2-\alpha]\sinh[\mathrm{i}(\mu-v)/2+\alpha]}. \tag{2.87}$$

This can be seen to be true if we rewrite (2.26) using (2.25) as

$$\lambda^2(k) = (c'r(k)+b)(c/r(k)+b) \tag{2.88}$$

then use (2.55) and (2.71).

Hence

$$f_N = -\frac{kT}{N}\sum_{j=1}^{n} \ln \psi(\alpha_j). \tag{2.89}$$

In the thermodynamic limit we have

$$f_\infty = -kT\int_0^\infty \ln \psi(\alpha)\rho_\infty(\alpha)\,\mathrm{d}\alpha. \tag{2.90}$$

In appendix 1 we also solve (2.90) to find the known result (Baxter 1982)

$$f_\infty = -kT\int_{-\infty}^{\infty} \frac{\sinh(2vy)\sinh[(\pi-\mu)y]\,\mathrm{d}y}{2y\sinh(\pi y)\cosh(\mu y)}. \tag{2.91}$$

3. Finite-size corrections

In this section we take the Bethe ansatz equations and our expressions for the free energy and, using the technique described in Hamer *et al* (1987), calculate the surface free energy as the first-order correction to the bulk limit. We find the second-order correction which gives us the conformal anomaly.

We begin by writing the expressions for the density of roots and the free energy for finite N, using the definitions (2.80) and (2.89), as

$$\rho_N(\alpha) = \frac{1}{2\pi}\left[\phi'\left(\alpha, \frac{\mu-v}{2}\right) + \phi'\left(\alpha, \frac{\mu+v}{2}\right)\right] + \frac{1}{2\pi N}[\phi'(2\alpha,\mu)+\phi'(\alpha,\mu)]$$
$$-\frac{1}{2\pi N}\sum_{l=-n}^{n} \phi'(\alpha-\alpha_l,\mu) \tag{3.1}$$

and

$$\frac{-f_N}{kT}=\int_{-\infty}^{\infty}\xi(\alpha)\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)\right)\mathrm{d}\alpha-\frac{\xi(0)}{N} \tag{3.2}$$

where

$$\xi(\alpha)=\ln\left(\frac{\sinh\{\mathrm{i}[(\mu+v)/2]-\alpha\}}{\sinh\{\mathrm{i}[(\mu-v)/2]+\alpha\}}\right). \tag{3.3}$$

Following de Vega and Woynarovich (1985) and Hamer *et al* (1987) we find expressions for the finite-size corrections in appendix 2. These are

$$\rho_N(\alpha)-\rho_\infty(\alpha)=\int_{-\infty}^{\infty}\frac{p(\alpha-\beta)}{\pi}\left(\frac{1}{N}\sum_{l=-n}^{n}\delta(\beta-\alpha_l)-\rho_N(\beta)\right)\mathrm{d}\beta+\frac{1}{\pi N}[p_2(\alpha)+p(\alpha)] \tag{3.4}$$

where

$$p(\alpha)=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\sinh[(\pi-2\mu)x/2]\,\mathrm{e}^{-\mathrm{i}\alpha x}\,\mathrm{d}x}{\sinh[(\pi-2\mu)x/2]+\sinh\pi x/2} \tag{3.5}$$

and

$$p_2(\alpha)=\int_{-\infty}^{\infty}\frac{\sinh[(\pi-2\mu)x/4]\cosh(\pi x/4)\,\mathrm{e}^{-\mathrm{i}\alpha x}\,\mathrm{d}x}{\sinh[(\pi-2\mu)x/2]+\sinh(\pi x/2)} \tag{3.6}$$

for the root density and

$$\frac{-(f_N-f_\infty)}{kT}=\int_{-\infty}^{\infty}F(\beta)\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\beta-\alpha_j)-\rho_N(\beta)\right)\mathrm{d}\beta-\frac{\xi(0)}{N}+\frac{1}{N}\int_{-\infty}^{\infty}\frac{\xi(\beta)}{\pi}[p_2(\beta)+p(\beta)]\,\mathrm{d}\beta \tag{3.7}$$

where

$$F(\alpha)=\xi(\alpha)-\int_{-\infty}^{\infty}\frac{\xi(\beta)}{\pi}\rho(\beta-\alpha)\,\mathrm{d}\beta \tag{3.8}$$

for the free energy. We evaluate $F(\alpha)$ via Fourier transforms in appendix 2 to give

$$F^{\mathrm{E}}(\alpha)=\tfrac{1}{2}\ln\left(\frac{\cosh(\pi\alpha/\mu)+\sin(\pi v/2\mu)}{\cosh(\pi\alpha/\mu)-\sin(\pi v/2\mu)}\right) \tag{3.9}$$

where $F^{\mathrm{E}}(\alpha)$ denotes the even part of $F(\alpha)$.

To evaluate (3.4) and (3.7) Woynarovich and Eckle (1987) introduced the Euler-Maclaurin formula which states (Hamer *et al* 1987) that if

$$S_N(\alpha)\equiv\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)-\rho_N(\alpha) \tag{3.10}$$

then

$$\int_{-\infty}^{\infty}g(\alpha)S_N(\alpha)\,\mathrm{d}\alpha \approx -\left(\int_{-\infty}^{-A}\mathrm{d}\alpha+\int_{A}^{\infty}\mathrm{d}\alpha\right)g(\alpha)\rho_N(\alpha)+\frac{1}{2N}[g(A)+g(-A)]+\frac{1}{12N^2\rho_N(A)}[g'(A)-g'(-A)] \tag{3.11}$$

for an arbitrary function $g(\alpha)$ analytic in $[-A, A]$, where A is the largest root, determined by

$$Z_N(A) = n/N = \tfrac{1}{2}. \tag{3.12}$$

Applying (3.11) to (3.4) and (3.7) we have for the root density

$$\begin{aligned}\rho_N(\alpha) - \rho_\infty(\alpha) &= \int_A^\infty \frac{\rho_N(\beta)}{\pi} p(\alpha-\beta)\,\mathrm{d}\beta - \frac{1}{2\pi N} p(\alpha - A) \\ &\quad + \frac{p'(\alpha - A)}{12\pi N^2 \rho_N(A)} + \frac{1}{\pi N}[p_2(\alpha) + p(\alpha)] + \text{terms smaller in } N \end{aligned} \tag{3.13}$$

and for the free energy

$$\begin{aligned}\frac{-(f_N - f_\infty)}{kT} &= -2\int_A^\infty F(\beta)\rho_N(\beta)\,\mathrm{d}\beta + \frac{F(A)}{N} + \frac{F'(A)}{6N^2\rho_N(A)} - \frac{\xi(0)}{N} \\ &\quad + \int_{-\infty}^{\infty} \frac{\xi(\beta)}{N}[p_2(\beta) + p(\beta)]\,\mathrm{d}\beta. \end{aligned} \tag{3.14}$$

It can be seen that (3.13) is an integral equation of the Wiener-Hopf type and can be treated in a similar way to Hamer *et al* (1987). This has been done in appendix 3. The result has then been used in (3.14) in appendix 3 to achieve the conclusion:

$$\begin{aligned} f_N - f_\infty &= \frac{kT}{N}\bigg[\ln\left(\frac{\sin[(\mu+v)/2]}{\sin[(\mu-v)/2]}\right) \\ &\quad - \int_{-\infty}^{\infty} \frac{2\sinh(vy)\sinh[(\pi-2\mu)y/2]\cosh[(\pi-\mu)y/2]\cosh(\mu y/2)}{y\sinh(\pi y)\cosh(\mu y)}\,\mathrm{d}y\bigg] \\ &\quad + \frac{kT}{N^2}\left[-\frac{\pi}{12}\tan\left(\frac{\pi v}{2\mu}\right)\left(1 - \frac{6\mu^2}{\pi(\pi-\mu)}\right)\right]. \end{aligned} \tag{3.15}$$

This formula provides the finite-size corrections to the free energy of our model up to second order. This result is discussed in the next section.

4. Conformal invariance

In two dimensions the group of conformal transformations is isomorphic to the group of analytic functions and so is of infinite dimensionality. Conformal invariance therefore provides large restrictions on the form of mathematical models in two dimensions. Conformal invariance (for a review see Cardy 1987) has been hypothesised to hold in critical statistical mechanics lattice systems (and critical quantum spin chains).

It has been shown that conformal invariance (Blöte *et al* 1986, Affleck 1986) predicts the form of the finite-size corrections to the free energy:

$$f_{N'} = f_\infty + \frac{s_\infty}{N'} - \frac{\pi\zeta c}{24N'^2} + o(N'^{-2}) \tag{4.1}$$

for free boundary conditions where s_∞ is the surface free energy, c is the conformal anomaly which governs the critical exponents of the system and ζ is a scale factor independent of boundary conditions.

We can immediately identify the surface free energy from (3.15) as

$$s_\infty = \tfrac{1}{2}\ln\left(\frac{\sin[(\mu+v)/2]}{\sin[(\mu-v)/2]}\right) - \int_{-\infty}^{\infty} \frac{\sinh(vy)\sinh[(\pi-2\mu)y]\cosh[(\pi-\mu)y/2]\cosh(\mu y/2)\,\mathrm{d}y}{y\sinh(\pi y)\cosh(\mu y)}. \tag{4.2}$$

The conformal anomaly can be extracted in comparison with previous results (Hamer *et al* 1987) as

$$c = 1 - \frac{6\mu^2}{\pi(\pi-\mu)}. \tag{4.3}$$

This leaves the scale factor as

$$\zeta \equiv \zeta_d = \tfrac{1}{2}\tan(\pi v/2\mu) \tag{4.4}$$

(remembering $2N' = N$).

For a lattice with the standard orientation, de Vega and Karowski (1987) obtain

$$\zeta_n = \sin(\pi v/\mu). \tag{4.5}$$

This difference can be explained using conformal invariance (Kim and Pearce 1987). Cardy (1987) explains that conformal invariance implies scale, translational and rotational invariances. Neither the system of de Vega and Karowski (1987) or our system are rotationally invariant (unless $v = \mu/2$). This problem disappears if we shear the lattice to effectively rescale in one direction, so obtaining rotational invariance. This involves the 'isotropy angle' θ (Kim and Pearce 1987) as a 'natural' shear angle. After shearing by this angle the two systems should be equivalent.

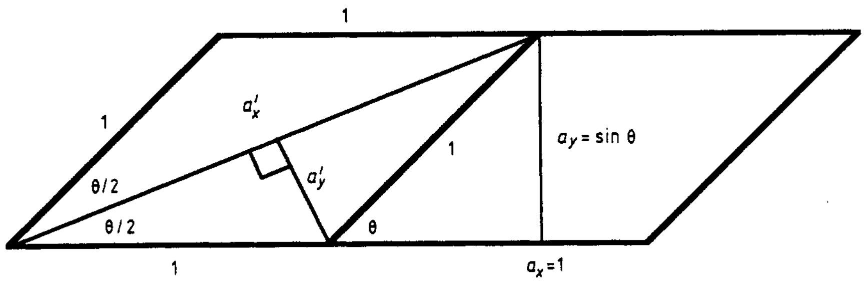

Figure 4. This diagram pictures two faces of a lattice sheared by the isotropy angle θ, which ensures rotational invariance. The scale factors for the normal square lattice and for the rotated lattice are calculated as the ratios of the respective 'vertical' to 'horizontal' single lattice spacings, where $\theta = \pi v/\mu$, so

$$\zeta_n = \frac{a_y}{a_x} = \sin(\pi v/\mu)$$

and

$$\zeta_d = \frac{a'_y}{a'_x} = \frac{\sin(\pi v/2\mu)}{2\sin(\pi/2 - \pi v/2\mu)} = \tfrac{1}{2}\tan(\pi v/2\mu).$$

The scale factor in each case can be calculated by taking the ratio of the two perpendicular single-lattice face distances that are relevant to the orientation of the system in question. One is in the direction in which the transfer matrix acts and the other is parallel to the row on which the transfer matrix acts (figure 4). Therefore we have

$$\zeta_n = a_y/a_x = \sin(\pi v/\mu) \tag{4.6a}$$

and

$$\zeta_d = a'_y/a'_x = \tfrac{1}{2}\tan(\pi v/2\mu). \tag{4.6b}$$

We use $\theta = \pi v/\mu$ in calculating these ratios and this gives us the two scale factors.

Hence, even though ζ is independent of boundary conditions, it is dependent on the orientation of the lattice (i.e. how one chooses the transfer matrix). Our scale factor ζ_d is then explained using the rotational invariance needed for the conformal theory to hold.

5. Summary

We have written down the Bethe ansatz equation (2.74) for a six-vertex model on a lattice of rotated orientation with general boundary weights and obtained the large-N solution. The equations simplify if (2.60) is imposed on the boundary weights, and this case is of interest as it includes the Potts model with free boundaries, when the boundary weights are given by (2.66). We have then calculated the finite-size corrections (3.15) to the free energy. In particular, these give the surface free energy (4.2), the conformal anomaly (4.3) and scale factor ζ (4.4). This scale factor ζ differs from that of a non-rotated lattice: it is explained using a geometric argument assuming conformal invariance.

Acknowledgment

The authors thank M N Barber and C J Hamer for illuminating discussions and G R W Quispel for his kind assistance and comments.

Appendix 1. The thermodynamic limit of the Bethe ansatz equations

In this appendix we solve the integral equations (2.81) and (2.90) to find the limiting root density $\rho_\infty(\alpha)$ and the free energy f_∞.

We begin by defining Fourier transform pairs (which will be used throughout the appendices) as

$$\bar{f}(x) = \int_{-\infty}^{\infty} f(\alpha)\, e^{i\alpha x}\, d\alpha \tag{A1.1a}$$

and

$$f(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \bar{f}(x)\, e^{-i\alpha x}\, dx. \tag{A1.1b}$$

We restate (2.87) as

$$\rho_\infty(\alpha)=\frac{1}{2\pi}\left[\phi'\left(\alpha,\frac{\mu-v}{2}\right)+\phi'\left(\alpha,\frac{\mu+v}{2}\right)\right]-\frac{1}{2\pi}\int_{-\infty}^{\infty}\rho_\infty(\beta)\phi'(\alpha-\beta,\mu)\,\mathrm{d}\beta \tag{A1.2}$$

where

$$\phi'(\alpha,\mu)=\frac{2\sin 2\mu}{\cosh 2\alpha-\cos 2\mu}. \tag{A1.3}$$

We apply the Fourier transform to (A1.2), using the integral, which can be done by contour integration:

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\sin\mu\,\mathrm{e}^{\mathrm{i}\alpha x}}{\cosh 2\alpha-\cos\mu}\,\mathrm{d}\alpha=\frac{\sinh[(\pi-\mu)x/2]}{\sinh(\pi x/2)}. \tag{A1.4}$$

We solve for $\bar{\rho}_\infty(x)$ as

$$\bar{\rho}_\infty(x)=\frac{\cosh(vx/2)}{\cosh(\mu x/2)}. \tag{A1.5}$$

Again, using contour integration we know

$$\int_{-\infty}^{\infty}\frac{\mathrm{e}^{ax}}{\cosh x}\,\mathrm{d}x=\frac{\pi}{\cos(\pi a/2)}\qquad |\mathrm{Re}\,a|<1 \tag{A1.6}$$

so

$$\rho_\infty(\alpha)=\frac{2\cos(\pi v/2\mu)\cosh(\pi\alpha/\mu)}{\mu[\cosh(2\pi\alpha/\mu)+\cos(\pi v/\mu)]} \tag{A1.7}$$

as given in (2.83).

We can now examine the free energy f_∞. It is given by recasting (2.90) as

$$f_\infty=-kT\int_{-\infty}^{\infty}\xi(\alpha)\rho_\infty(\alpha)\,\mathrm{d}\alpha \tag{A1.8}$$

where

$$\xi(\alpha)=\ln\left(\frac{\sinh\{\mathrm{i}[(\mu+v)/2]-\alpha\}}{\sinh\{\mathrm{i}[(\mu-v)/2]+\alpha\}}\right). \tag{A1.9}$$

We now use a corollary of the convolution theorem of Fourier transforms that states if $\bar{f}(x)$ (respectively $\bar{g}(x)$) is the transform of $f(\alpha)$ (respectively $g(\alpha)$) then

$$\int_{-\infty}^{\infty}f(\alpha)g(-\alpha)\,\mathrm{d}\alpha=\frac{1}{2\pi}\int_{-\infty}^{\infty}\bar{f}(x)\bar{g}(x)\,\mathrm{d}x. \tag{A1.10}$$

Then, applying (A1.10) to (A1.8) it is found that

$$f_\infty=-kT\int_{-\infty}^{\infty}\frac{\bar{\xi}(x)}{2\pi}\bar{\rho}_\infty(x)\,\mathrm{d}x. \tag{A1.11}$$

It is only left to evaluate $\bar{\xi}(x)/2\pi$ but we need only calculate the even part of this as only the even part contributes to the integral since $\bar{\rho}_\infty(x)$ is even. Now

$$\frac{\bar{\xi}^{-\mathrm{E}}(x)}{2\pi}=\text{even part}\left(\int_{-\infty}^{\infty}\frac{\xi(\alpha)}{2\pi}\mathrm{e}^{\mathrm{i}\alpha x}\,\mathrm{d}\alpha\right) \tag{A1.12}$$

$$=\text{even part}\left(-\int_{-\infty}^{\infty}\frac{\xi'(\alpha)}{2\pi\mathrm{i}x}\mathrm{e}^{\mathrm{i}\alpha x}\,\mathrm{d}\alpha\right) \tag{A1.13}$$

where

$$\xi'(\alpha)=\frac{2\mathrm{i}\sin\mu}{\cosh(2\alpha-\mathrm{i}v)-\cos\mu}. \tag{A1.14}$$

We use the integral

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\sin\mu\,\mathrm{e}^{\mathrm{i}\alpha x}}{\cosh(2\alpha-\mathrm{i}v)-\cos\mu}\,\mathrm{d}\alpha=\frac{\mathrm{e}^{-vx/2}\sinh[(\pi-\mu)x/2]}{\sinh(\pi x/2)} \tag{A1.15}$$

evaluated by contour integration, to show

$$\frac{\bar{\xi}^{\mathrm{E}}(x)}{2\pi}=\frac{\sinh(vx/2)\sinh[(\pi-\mu)x/2]}{\sinh(\pi x/2)}. \tag{A1.16}$$

The result required in (2.91) is then obtained by making the substitution $2y=x$.

Appendix 2. Finite-size correction equations

In this appendix we provide the derivation of the finite-size correction equations.

We consider (3.1) and (2.80) to give

$$\begin{aligned}\rho_N(\alpha)-\rho_\infty(\alpha)&=\int_{-\infty}^{\infty}\frac{\phi'(\alpha-\beta,\mu)}{2\pi}\left(\rho_\infty(\beta)-\frac{1}{N}\sum_{j=-n}^{n}\delta(\beta-\alpha_j)\right)\mathrm{d}\beta\\&\quad+\frac{1}{2\pi N}[\phi'(2\alpha,\mu)+\phi'(\alpha,\mu)] \qquad\qquad (\mathrm{A2.1})\\&=\int_{-\infty}^{\infty}\frac{\phi'(\alpha-\beta,\mu)}{2\pi}\left(\rho_N(\beta)-\frac{1}{N}\sum_{j=-n}^{n}\delta(\beta-\alpha_j)\right)\mathrm{d}\beta\\&\quad-\int_{-\infty}^{\infty}\frac{\phi'(\alpha-\beta,\mu)}{2\pi}[\rho_N(\beta)-\rho_\infty(\beta)]\,\mathrm{d}\beta+\frac{1}{2\pi N}[\phi'(2\alpha,\mu)+\phi'(\alpha,\mu)]. \qquad (\mathrm{A2.2})\end{aligned}$$

This can now be solved for $\rho_N(\alpha)-\rho_\infty(\alpha)$ via Fourier transforms to obtain

$$\begin{aligned}\bar{\rho}_N(x)-\bar{\rho}_\infty(x)&=-\frac{\overline{\phi'}(x,\mu)/2\pi}{1+\overline{\phi'}(x,\mu)/2\pi}\left[\int_{-\infty}^{\infty}\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\beta-\alpha_j)-\rho_N(\beta)\right)\mathrm{e}^{\mathrm{i}x\beta}\,\mathrm{d}\beta\right]\\&\quad+\frac{1}{N}\left(\frac{\overline{\phi'}(x/2,\mu)/2\pi}{1+\overline{\phi'}(x,\mu)/2\pi}+\frac{\overline{\phi'}(x,\mu)/2\pi}{1+\overline{\phi'}(x,\mu)/2\pi}\right).\end{aligned} \tag{A2.3}$$

This gives the result (3.4) with (3.5) and (3.6) defined as

$$\bar{\rho}(x)=\frac{1}{2}\,\frac{\overline{\phi'}(x,\mu)/2\pi}{1+\overline{\phi'}(x,\mu)/2\pi} \tag{A2.4}$$

and

$$\bar{\rho}_2(x)=\frac{1}{2}\,\frac{\overline{\phi'}(x/2,\mu)/2\pi}{1+\overline{\phi'}(x,\mu)/2\pi}. \tag{A2.5}$$

Next, we obtain from (2.90) and (3.3)

$$\frac{-(f_N-f_\infty)}{kT}=\int_{-\infty}^{\infty}\xi(\alpha)\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)-\rho_\infty(\alpha)\right)\mathrm{d}\alpha-\frac{\xi(0)}{N} \tag{A2.6}$$

$$=\int_{-\infty}^{\infty}\xi(\alpha)\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)-\rho_N(\alpha)\right)\mathrm{d}\alpha-\frac{\xi(0)}{N}$$
$$+\int_{-\infty}^{\infty}\xi(\alpha)(\rho_N(\alpha)-\rho_\infty(\alpha))\,\mathrm{d}\alpha. \tag{A2.7}$$

Substituting (3.4) into (A2.7) we find

$$\frac{-(f_N-f_\infty)}{kT}=\int_{-\infty}^{\infty}\xi(\alpha)\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)-\rho_N(\alpha)\right)\mathrm{d}\alpha-\frac{\xi(0)}{N}$$
$$-\int_{-\infty}^{\infty}\left(\frac{1}{N}\sum_{j=-n}^{n}\delta(\beta-\alpha_j)-\rho_N(\beta)\right)\int_{-\infty}^{\infty}\frac{\xi(\alpha)}{\pi}p(\alpha-\beta)\,\mathrm{d}\alpha\,\mathrm{d}\beta$$
$$-\int_{-\infty}^{\infty}\frac{\xi(\alpha)}{\pi N}(p_2(\alpha)+p(\alpha))\,\mathrm{d}\alpha. \tag{A2.8}$$

This is the result (3.7).

It is left to evaluate (3.8) by Fourier transforms so

$$F^{\mathrm{E}}(\alpha)=\int_{-\infty}^{\infty}\frac{\sinh(vx/2)\,\mathrm{e}^{-\mathrm{i}\alpha x}}{2x\cosh(\mu x/2)}\,\mathrm{d}x \tag{A2.9}$$

where, again we are only interested in the even part of $F(\alpha)$ since the rest of the integrand in (3.7) is even. We can evaluate (A2.9) by noting that

$$F^{\mathrm{E}'}(\alpha)=-\mathrm{i}\int_{-\infty}^{\infty}\frac{\sinh(vx/2)\,\mathrm{e}^{-\mathrm{i}\alpha x}}{2\cosh(\mu x/2)}\,\mathrm{d}x. \tag{A2.10}$$

Using

$$\int_{-\infty}^{\infty}\frac{\mathrm{e}^{ax}\,\mathrm{d}x}{\cosh x}=\frac{\pi}{\cos(\pi a/2)}\qquad |\mathrm{Re}\,a|<1 \tag{A2.11}$$

we find

$$F^{\mathrm{E}'}(\alpha)=\frac{-2\pi}{\mu}\frac{\sin(\pi v/2\mu)\sinh(\pi\alpha/\mu)}{[\cosh(2\pi\alpha/\mu)+\cos(\pi v/\mu)]}. \tag{A2.12}$$

The required result (3.9) can be found from (A2.12) using the indefinite integral

$$\int^{z}\frac{\mathrm{d}z}{z^2-a^2}=\frac{1}{2a}\ln\left(\frac{z-a}{z+a}\right) \tag{A2.13}$$

after substituting $z=\cosh(\pi\alpha/\mu)$.

Appendix 3. Wiener–Hopf technique

In this appendix we apply the procedure explained by Hamer *et al* (1987) to solve (3.13) and so, in turn, (3.14) for the finite-size corrections to the free energy.

We will refer to equations of Hamer *et al* (1987) by using the prefix H. We begin with (3.13) by noting that using the definitions

$$K(\alpha)=p(\alpha)/\pi \tag{A3.1}$$

$$f(\alpha)=\rho_\infty(\alpha+A) \tag{A3.2}$$

$$\chi(\alpha)=\rho_N(\alpha+A) \tag{A3.3}$$

and setting $t=\alpha+A$ we can find an equation of the standard Wiener–Hopf type (H2.29):

$$\chi(t)-\int_0^\infty k(t-s)\chi(s)\,\mathrm{d}s=f(t)-\frac{1}{2N}k(t)+\frac{1}{12N^2\rho_N(A)}k'(t). \tag{A3.4}$$

This equation can be treated via the Fourier transforms defined in (A1.1). The kernel

$$(1-\bar{k}(x))=\frac{\sinh(\pi x/2)}{2\sinh[(\pi-\mu)x/2]\cosh(\mu x/2)} \tag{A3.5}$$

can be rewritten as the product of two functions $\bar{g}_\pm(x)$ that are holomorphic and continuous in the half-planes $\pi_\pm$ respectively. We have

$$(1-\bar{k}(x))^{-1}=\bar{g}_+(x)\bar{g}_-(x) \tag{A3.6}$$

where

$$\bar{g}_+(x)=\bar{g}_-(-x)=\frac{[2(\pi-\mu)]^{1/2}\Gamma(1-\mathrm{i}x/2)\mathrm{e}^{\psi(x)}}{\Gamma(\frac{1}{2}-\mathrm{i}\mu x/2\pi)\Gamma(1-\mathrm{i}(\pi-\mu)x/2\pi)} \tag{A3.7}$$

and $\psi(x)$ is given by

$$\psi(x)=\frac{\mathrm{i}x}{2}\left[\ln\left(\frac{\pi}{\pi-\mu}\right)-\frac{\mu}{\pi}\ln\left(\frac{\mu}{\pi-\mu}\right)\right]. \tag{A3.8}$$

The functions $\bar{\chi}(x)$ and $\bar{f}(x)$ can be split (as in (H2.40) and (H2.42)) into the sum of two functions holomorphic and continuous in the half-planes $\pi_\pm$ as

$$\bar{\chi}(x)=\bar{\chi}_+(x)+\bar{\chi}_-(x) \tag{A3.9}$$

where

$$\chi_\pm(t)=\begin{cases}\chi(t) & \text{for } t\gtrless 0\\ 0 & \text{for } t\lessgtr 0\end{cases} \tag{A3.10}$$

(and similarly for $\bar{f}(x)$).

An equation of identical form to (H2.43) is thus obtained:

$$\bar{\chi}_-(x)+(1-\bar{k}(x))(\bar{\chi}_+(x)-\bar{c}(x))=\bar{f}_+(x)+\bar{f}_-(x)-\bar{c}(x) \tag{A3.11}$$

where

$$\bar{c}(x)=\frac{1}{2N}+\frac{\mathrm{i}x}{12N^2\rho_N(A)}. \tag{A3.12}$$

We would like to separate (A3.11) into parts analytic in each half-plane. In doing this we define

$$\bar{g}_-(x)\bar{f}_+(x)=\bar{q}_+(x)+\bar{q}_-(x) \tag{A3.13}$$

similar to (H2.46).

So (A3.11) can be rewritten as

$$(\bar{\chi}_+(x)-\bar{c}(x))/\bar{g}_+(x)-\bar{q}_+(x)=\bar{q}_-(x)-\bar{g}_-(x)[\bar{\chi}_-(x)+\bar{c}(x)-\bar{f}(x)]\equiv\bar{r}(x) \tag{A3.14}$$

which is identical in form to (H2.47).

The argument from Hamer *et al* (1987) then becomes that the two sides of (A3.14) are analytic in different half-planes, but because there is a common strip of regularity including the junction of the half-planes $\pi_\pm$, one side must be the analytic continuation of the other. Hence $\bar{r}(x)$ is entire and can be determined from its asymptotic behaviour.

Now using the asymptotic expansions (H2.48) we find

$$\bar{r}(x)=\frac{-g}{144N^2\rho_N(A)}-\frac{1}{2N}-\frac{\mathrm{i}x}{12N^2\rho_N(A)} \tag{A3.15}$$

where

$$g=2+\frac{\pi}{\mu}-\frac{2\pi}{\pi-\mu}. \tag{A3.16}$$

The first significant departure from the analysis of Hamer *et al* (1987) appears now when we evaluate $\bar{f}(x)$ as

$$\bar{f}(x)=\frac{\mathrm{e}^{-\mathrm{i}xA}\cosh(vx/2)}{\cosh(\mu x/2)} \qquad |v|<\mu \tag{A3.17}$$

and keeping the leading pole term in π_- we have

$$\bar{f}(x)\approx\frac{2\,\mathrm{e}^{-\mathrm{i}xA}\cosh(vx/2)}{(\pi-\mathrm{i}\mu x)}. \tag{A3.18}$$

Following Hamer *et al* (1987) we can estimate

$$\bar{q}_+(x)=\frac{2\bar{g}_+(\mathrm{i}\pi/\mu)\,\mathrm{e}^{-\pi A/\mu}\cosh(-\mathrm{i}\pi v/2\mu)}{(\pi-\mathrm{i}\mu x)}. \tag{A3.19}$$

We now have all we need to find $\chi_+(x)$ as

$$\bar{\chi}_+(x)=\int_0^\infty \mathrm{e}^{\mathrm{i}xt}\chi(t)\,\mathrm{d}t=\bar{c}(x)+\bar{g}_+(x)[\bar{r}(x)+\bar{q}_+(x)]. \tag{A3.20}$$

We now return to the determination of A via (3.12). Firstly, we know that

$$\begin{aligned}\int_{-\infty}^{\infty}\rho_N(\alpha)\,\mathrm{d}\alpha&=\lim_{\eta\to\infty}2Z_N(\eta)\\&=1+\frac{1}{N}\left(1-\frac{2\mu}{\pi}\right)\end{aligned} \tag{A3.21}$$

but (3.12) implies

$$\int_{-A}^{A}\rho_N(\alpha)\,\mathrm{d}\alpha=1 \tag{A3.22}$$

so

$$\int_A^\infty\rho_N(\alpha)\,\mathrm{d}\alpha=\frac{1}{2N}\left(1-\frac{2\mu}{\pi}\right). \tag{A3.23}$$

Now, when $x=0$ in (A3.20) we have

$$\int_A^\infty \rho_N(\alpha)\,\mathrm{d}\alpha = \frac{1}{2N} + \bar{g}_+(0)[\bar{r}(0) + \bar{q}_+(0)] \tag{A3.24}$$

and combining (A3.23) and (A3.24) it can be shown that

$$\bar{q}_+(0) = -\bar{r}(0) - \frac{\mu}{\pi N \bar{g}_+(0)} \tag{A3.25}$$

i.e.

$$\frac{2}{\pi}\bar{g}_+(\mathrm{i}\pi/\mu)\,\mathrm{e}^{-\pi A/\mu}\cos(\pi v/2\mu) = \frac{1}{2N} + \frac{g}{144N^2\rho_N(A)} - \frac{\mu}{\pi N\bar{g}_+(0)}. \tag{A3.26}$$

By contour integration we obtain

$$\begin{aligned}\rho_N(A) = 2\bar{\psi}_+(0) &= \frac{1}{\pi}\int_{-\infty}^{\infty} \bar{\chi}(x)\,\mathrm{d}x \\ &= -\frac{g^2}{384N^2\rho_N(A)} - \frac{\mathrm{i}g}{24N} + \frac{\bar{g}_+(\mathrm{i}\pi/\mu)\,\mathrm{e}^{-\pi A/\mu}\cos(\pi v/2\mu)}{\mu}.\end{aligned} \tag{A3.27}$$

Defining $\rho = 4N^2 r_N(A)$ combined with (A3.26) and (A3.27) it can be shown that ρ satisfies the quadratic

$$\rho^2 + \left(\frac{g}{6} - \frac{2\pi}{\mu} - \frac{4\pi\alpha}{\mu}\right)\rho + \left(\frac{g^2}{216} - \frac{\pi g}{9\mu}\right) = 0 \tag{A3.28}$$

where

$$\alpha = -\mu/\pi\bar{g}_+(0). \tag{A3.29}$$

We are now in a position to examine (3.14) although we first note that $F(\alpha)$ behaves like

$$F(\alpha) \approx 2\sin\left(\frac{\pi v}{2\mu}\right)\mathrm{e}^{-\pi\alpha/\mu} \qquad \text{for } \alpha \text{ large.} \tag{A3.30}$$

We first examine the terms

$$T_1 \equiv \int_A^\infty F(\beta)\rho_N(\beta)\,\mathrm{d}\beta - \frac{F(A)}{2N} - \frac{F'(A)}{12N^2\rho_N(A)} \tag{A3.31}$$

in (3.14).

From (A3.30) it follows that

$$T_1 = 2\sin\left(\frac{\pi v}{2\mu}\right)\mathrm{e}^{-\pi A/\mu}\left(\int_A^\infty \mathrm{e}^{-\pi(\beta-A)/\mu}\rho_N(\beta)\,\mathrm{d}\beta - \frac{1}{2N} - \frac{\pi}{12\mu N^2\rho_N(A)}\right) \tag{A3.32}$$

$$= 2\sin\left(\frac{\pi v}{2\mu}\right)\mathrm{e}^{-\pi A/\mu}\left[\bar{\chi}_+\left(\frac{\mathrm{i}\pi}{\mu}\right) - c\left(\frac{\mathrm{i}\pi}{\mu}\right)\right] \tag{A3.33}$$

so from (A3.20)

$$T_1 = 2\sin\left(\frac{\pi v}{2\mu}\right)\mathrm{e}^{-\pi A/\mu}\bar{g}_+\left(\frac{\mathrm{i}\pi}{\mu}\right)\left[\bar{r}\left(\frac{\mathrm{i}\pi}{\mu}\right) + \bar{q}_+\left(\frac{\mathrm{i}\pi}{\mu}\right)\right]. \tag{A3.34}$$

Using the definitions of $\bar{r}(x)$ and $\bar{q}_+(x)$ and the fact that $\bar{q}_+(\mathrm{i}\pi/\mu)=\frac{1}{2}\bar{q}_+(0)$, along with (A3.26) and finally (A3.28), we arrive at the conclusion that

$$T_1=-\frac{\pi}{24N^2}\tan\left(\frac{\pi v}{2\mu}\right)(1-12\alpha^2) \tag{A3.35}$$

where

$$\alpha=\frac{-\mu}{[2\pi(\pi-\mu)]^{1/2}}. \tag{A3.36}$$

Secondly, we examine the rest of the terms as

$$T_2\equiv\frac{\xi(0)}{N}-\int_{-\infty}^{\infty}\frac{\xi(\beta)}{N}[p_2(\beta)+p(\beta)]\,\mathrm{d}\beta. \tag{A3.37}$$

We simply rewrite T_2 using the same procedure of Fourier transforming the integrand we used to express the free energy in appendix 1. This results in

$$T_2=\frac{\xi(0)}{N}-\int_{-\infty}^{\infty}\frac{\sinh(vx/2)\sinh[(\pi-2\mu)x/4]\cosh[(\pi-\mu)x/4]\cosh(\mu x/4)\,\mathrm{d}x}{Nx\sinh(\pi x/2)\cosh(\mu x/2)}. \tag{A3.38}$$

Combining (A3.35) and (A3.38) the result (3.15) follows.

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