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1987 J. Phys. A: Math. Gen. 20 6397

(http://iopscience.iop.org/0305-4470/20/18/038)

J. Phys. A: Math. Gen. **20** (1987) 6397-6409. Printed in the UK

Surface exponents of the quantum *XXZ*, Ashkin–Teller and Potts models

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Received 20 March 1987

Abstract. Eigenspectra of the critical quantum Ashkin-Teller and Potts chains with free boundaries can be obtained from that of the *XXZ* chain with free boundaries and a complex surface field. By deriving and solving numerically the Bethe ansatz equations for such boundaries we obtain eigenenergies of *XXZ* chains of up to 512 sites. The conformal anomaly and surface exponents of the quantum *XXZ*, Ashkin-Teller, and Potts chains are calculated by exploiting their relations with the mass gap amplitudes as predicted by conformal invariance.

1. Introduction

Statistical mechanical systems with short-range interactions are believed to be conformally invariant at criticality (Polyakov 1970, Belavin *et al* 1984). In two dimensions this assumption has many significant implications (for a review see Cardy (1987)). In particular, the mass gap amplitudes associated with the asymptotically merging levels in the eigenvalue spectrum of the transfer matrix, or associated Hamiltonian, in a finite strip are related to the anomalous dimensions of the operators describing the critical behaviour of the infinite system (Cardy 1984a, 1986a). Using these relations the critical exponents of the three-state Potts model (von Gehlen *et al* 1986, von Gehlen and Rittenberg 1986a, b), four-state Potts and Ashkin-Teller models (Alcaraz and Drugowich de Felício 1984, von Gehlen *et al* 1986, von Gehlen and Rittenberg 1986c, 1987) have been calculated from the eigenspectra of chains of length up to 10-13 sites, depending on the model.

Recently, Alcaraz *et al* (1987a, b) showed that the eigenspectrum of both the quantum Ashkin-Teller (Kohmoto *et al* 1981) and q-state Potts Hamiltonians on chains of M sites, with periodic or twisted boundary conditions, can be obtained exactly at criticality from the eigenspectrum of a $2M$-site quantum *XXZ* chain with appropriate boundary conditions. By numerically solving the Bethe ansatz equations for the eigenenergies of the *XXZ* chain they were able to calculate mass gap amplitudes in

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0305-4470/87/186397+16$02.50

the Ashkin-Teller and Potts models for chains up to 512 sites, thereby considerably improving previous numerical estimates of the bulk critical exponents and allowing an examination of the dominant finite-size corrections.

In this paper we consider the quantum Ashkin-Teller and Potts chains with free boundaries. The XXZ chain appropriate for our analysis is defined by the Hamiltonian (Alcaraz *et al* 1987a, b)

$$H_{XXZ} = -\tfrac{1}{2}\left(\sum_{j=1}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z) + i\alpha(\sigma_1^z - \sigma_L^z) \right) \tag{1.1}$$

where σ_i^x, σ_i^y, σ_i^z are Pauli matrices, $\Delta = -\cos\gamma$ and $\alpha = \sin\gamma$ are coupling constants with $\gamma \in [0, \pi)$. We observe that although the Hamiltonian (1.1) is not Hermitian the eigenenergies are real since (1.1) is invariant under complex conjugation and reflection symmetry (relabelling sites from right to left). The eigenenergies of the above Hamiltonian with $L = 2M$ sites and free ends ($\alpha = 0$) are exactly related (Alcaraz *et al* 1987a, b) to those of the self-dual M-site quantum Ashkin-Teller chain with Hamiltonian (Kohmoto *et al* 1981)

$$H_{AT} = -\tfrac{1}{2} \sum_{i=1}^{M} (\sigma_i^z \sigma_{i+1}^z + \tau_i^z \tau_{i+1}^z + \lambda \sigma_i^z \sigma_{i+1}^z \tau_i^x \tau_{i+1}^x + \sigma_i^z + \tau_i^z + \lambda \sigma_i^x \sigma_i^x). \tag{1.2}$$

Here σ_i^z, σ_i^x and τ_i^z, τ_i^x are two commuting sets of Pauli matrices ($\sigma_{L+1}^z = \tau_{L+1}^x = 0$). As in the XXZ chain, $\lambda = \cos\gamma$, $\gamma \in [0, \pi]$ is a coupling constant and in the bulk limit the model is massless with a line of continuously varying exponents. When a temperature-like variable is introduced in (1.2) the phase diagram exhibits, apart from ferromagnetic and paramagnetic phases, a massless disordered phase. The region $-1/\sqrt{2} \leqslant \lambda \leqslant 1$ describes the critical surface separating the ferromagnetic and paramagnetic phases while $-1 \leqslant \lambda \leqslant -1/\sqrt{2}$ are points inside a massless critical phase (Kohmoto *et al* 1981).

On the other hand the eigenenergies of a $2M$-site XXZ Hamiltonian (1.1), with couplings $\gamma = \cos^{-1}(\sqrt{q}/2)$ ($q = 2, 3, 4$) are exactly related (Hamer 1981, Alcaraz *et al* 1987a, b) to the eigenenergies of an M-site self-dual q-state quantum Potts chain with free ends ($S_{L+1} = 0$), defined by the Hamiltonian

$$H_q = -\frac{1}{\sqrt{q}} \sum_{i=1}^{M} \sum_{k=0}^{q-1} (S_i^k S_{i+1}^{q-k} + R_i^k) + (2M-1)\sqrt{q}/4 \tag{1.3}$$

where S_i and R_i are $q \times q$ matrices satisfying the $Z(q)$ algebra

$$\begin{aligned} &[R_i, R_j] = [S_i, S_j] = [S_i, R_j] = 0 \qquad i \neq j \\ &S_j R_j = \exp(i2\pi/q) R_j S_j \qquad R_i^q = S_i^q = 1. \end{aligned} \tag{1.4}$$

For general values of γ, (1.1) describes the Hamiltonian analogue of the continuous ($0 \leqslant q \leqslant 4$) q-state Potts model (Alcaraz *et al* 1987a, b).

The Bethe ansatz equations for the Hamiltonian (1.1) with $\alpha = 0$ have been derived by Gaudin (1971, 1983). In the next section we derive Bethe ansatz equations for the free XXZ chain with an arbitrary 'surface' field at each end of the chain. By numerically solving these equations for the XXZ chain (1.1) we obtain eigenenergies, for M up to 256, of the quantum Ashkin-Teller (1.2) and Potts (1.3) chains. In this way accurate estimates are obtained in § 4 for the surface exponents of the models from the predictions of conformal invariance.

2. Bethe ansatz

Rather than directly considering the Hamiltonian (1.1), we define a more general Hamiltonian by

$$H_{XXZ} = -\tfrac{1}{2}\left(\sum_{j=1}^{L-1}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\Delta\sigma_j^z\sigma_{j+1}^z)+p\sigma_1^z+p'\sigma_L^z\right) \tag{2.1}$$

where Δ, p and p' are arbitrary constants. Since this Hamiltonian commutes with the total spin operator $\Sigma\sigma^z$, the number of down spins n is a good quantum number. We therefore consider

$$H|n\rangle = E|n\rangle \tag{2.2}$$

where

$$|n\rangle = \sum f(x_1,\ldots,x_n)|x_1,\ldots,x_n\rangle. \tag{2.3}$$

Here the $x_1,\ldots,x_n$ denote the locations of the down spins on the chain, and the summation extends over all sets of the n increasing integers varying between 1 and L (see, e.g. Gaudin 1983, Baxter 1982, ch 8)

$$1 \leqslant x_1 < x_2 < \ldots < x_n \leqslant L. \tag{2.4}$$

2.1. $n=1$

For one down spin on the chain, the eigenvalue equation (2.2) gives

$$Ef(x) = -f(x-1)-f(x+1)-\tfrac{1}{2}[(L-5)\Delta+p+p']f(x) \qquad x=2,\ldots,L-1. \tag{2.5}$$

At the boundaries, we get slightly different equations

$$Ef(1) = -f(2)-\tfrac{1}{2}[(L-3)\Delta-p+p']f(1) \tag{2.6a}$$

$$Ef(L) = -f(L-1)-\tfrac{1}{2}[(L-3)\Delta+p-p']f(L). \tag{2.6b}$$

We now try as a solution

$$f(x) = A(k)\,e^{ikx} - A(-k)\,e^{-ikx}. \tag{2.7}$$

Substituting this in equation (2.5) we obtain the eigenvalue

$$E = -2\cos k - \tfrac{1}{2}[(L-5)\Delta+p+p']. \tag{2.8}$$

We want equation (2.5) to be valid for $x=1$ and $x=L$ also, where $f(0)$ and $f(L+1)$ are defined by (2.7). Combining (2.5) and (2.6) we get the end conditions

$$f(0) = (\Delta-p)f(1) \tag{2.9a}$$

$$f(L+1) = (\Delta-p')f(L). \tag{2.9b}$$

Defining the functions $\alpha(k)$ and $\beta(k)$ by

$$\alpha(k) = 1+(p-\Delta)\,e^{-ik} \tag{2.10a}$$

$$\beta(k) = [1+(p'-\Delta)\,e^{-ik}]\,e^{i(L+1)k} \tag{2.10b}$$

and substituting (2.7) in (2.9), we obtain

$$A(k)\alpha(-k)-A(-k)\alpha(k) = 0 \tag{2.11a}$$

$$A(k)\beta(k)-A(-k)\beta(-k) = 0. \tag{2.11b}$$

Compatibility between (2.11a) and (2.11b) yields

$$\alpha(k)\beta(k) = \alpha(-k)\beta(-k) \tag{2.12}$$

or, using (2.10),

$$e^{i2(L-1)k}\frac{(e^{ik}+p-\Delta)(e^{ik}+p'-\Delta)}{(e^{-ik}+p-\Delta)(e^{-ik}+p'-\Delta)}=1. \tag{2.13}$$

In the special case where the constants satisfy

$$(\Delta-p)(\Delta-p')=1 \tag{2.14}$$

(2.13) reduces to

$$e^{i2Lk}=1. \tag{2.15}$$

Given the compatibility relation (2.12), the solution of (2.11) for $A(k)$ is

$$A(k)=\beta(-k) \tag{2.16}$$

where it should be noted that $A(k)$ is determined up to a factor that is invariant under $k\leftrightarrow -k$.

2.2. $n=2$

For two down spins on the chain, we obtain the eigenvalue equation

$$\begin{aligned}Ef(x_1,x_2)=&-f(x_1-1,x_2)-f(x_1+1,x_2)-f(x_1,x_2-1)-f(x_1,x_2+1)\\&-\tfrac{1}{2}[(L-9)\Delta+p+p']f(x_1,x_2).\end{aligned} \tag{2.17}$$

We now also get the usual 'meeting condition' that arises because the two down spins may be neighbours (Gaudin 1983)

$$f(x_1,x_1)+f(x_1+1,x_1+1)-2\Delta f(x_1,x_1+1)=0. \tag{2.18}$$

In addition to this, as in the case $n=1$, we have two conditions to be satisfied at the free ends of the chain

$$f(0,x_2)=(\Delta-p)f(1,x_2) \tag{2.19a}$$

$$f(x_1,L+1)=(\Delta-p')f(x_1,L). \tag{2.19b}$$

Guided by the $n=1$ case we consider the ansatz

$$f(x_1,x_2)=\sum_P \varepsilon_P A(k_1,k_2)\,e^{i(k_1x_1+k_2x_2)} \tag{2.20}$$

where the sum extends over the permutations and the negations of k_1 and k_2, and ε_P is a sign factor (±1) that changes sign on negation or pair interchange. Substituting this ansatz in (2.17) we obtain the eigenvalue

$$E=-2\cos k_1-2\cos k_2-\tfrac{1}{2}[(L-9)\Delta+p+p']. \tag{2.21}$$

Defining the function $s(k_1,k_2)$ by

$$s(k_1,k_2)=1-2\Delta\,e^{ik_2}+e^{i(k_1+k_2)} \tag{2.22}$$

necessary conditions for the equations (2.18) and (2.19) to be satisfied are

$$A(k_1,k_2)s(k_1,k_2)-A(k_2,k_1)s(k_2,k_1)=0 \tag{2.23a}$$

$$A(k_1,k_2)\alpha(-k_1)-A(-k_1,k_2)\alpha(k_1)=0 \tag{2.23b}$$

$$A(k_1,k_2)\beta(k_2)-A(k_1,-k_2)\beta(-k_2)=0 \tag{2.23c}$$

together with nine other equations that can be obtained from (2.23) by applying permutations and negations. Using (2.23*a*), (2.23*c*), (2.23*a*) and (2.23*b*) 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 $A(k_1, k_2)$, the fact that the prefactor we pick up along the way is unity leads to

$$\frac{\alpha(k_1)\beta(k_1)}{\alpha(-k_1)\beta(-k_1)} = \frac{B(-k_1, k_2)}{B(k_1, k_2)} \tag{2.24}$$

where $B(k, k')$ is given by

$$B(k, k') = s(k, k')s(k', -k). \tag{2.25}$$

Using (2.10) we may rewrite the compatibility condition (2.24) as

$$e^{i2(L-1)k_1} \frac{(e^{ik_1}+p-\Delta)(e^{ik_1}+p'-\Delta)}{(e^{-ik_1}+p-\Delta)(e^{-ik_1}+p'-\Delta)} = \frac{B(-k_1, k_2)}{B(k_1, k_2)}. \tag{2.26}$$

Since there are eight functions that can be obtained from $A(k_1, k_2)$ by permutations and negations, it follows that there are eight compatibility equations to be satisfied, each analogous to (2.26). It is not difficult to see, however, that (2.26) is invariant under $k_1 \leftrightarrow -k_1$ and $k_2 \leftrightarrow -k_2$ (in fact, if $k_1 \neq 0$, (2.26) can be written as a polynomial equation in terms of $\cos k_1$ and $\cos k_2$ only), so permuting k_1 and k_2 results in just one more equation

$$\frac{\alpha(k_2)\beta(k_2)}{\alpha(-k_2)\beta(-k_2)} = \frac{B(-k_2, k_1)}{B(k_2, k_1)}. \tag{2.27}$$

Again in the special limit (2.14), there is some simplification in these equations, the left-hand sides of (2.24) and (2.27) reducing to $\exp(i2Lk_1)$ and $\exp(i2Lk_2)$, respectively.

In principle, the coupled equations (2.26) and (2.27) give k_1 and k_2 which in turn give the corresponding eigenvalue through (2.21). We now turn to the coefficient $A(k_1, k_2)$ in the wavefunction (2.20). From (2.23*a*) we have

$$A(k_1, k_2) = s(k_2, k_1)C(k_1, k_2) \tag{2.28}$$

where $C(k_1, k_2)$ is symmetric under $k_1 \leftrightarrow k_2$. In order to determine $C(k_1, k_2)$, we substitute (2.28) in (2.23*c*), obtaining

$$C(k_1, k_2) = \beta(-k_2)v(k_1, k_2)g(k_1) \tag{2.29}$$

where the symmetric function $v(k_1, k_2)$ is defined by

$$v(k_1, k_2) = e^{-ik_1} + e^{-ik_2} - 2\Delta. \tag{2.30}$$

The factor $g(k_1)$ is determined from the symmetry of $C(k_1, k_2)$ under $k_1 \leftrightarrow k_2$, resulting in

$$C(k_1, k_2) = \beta(-k_1)\beta(-k_2)v(k_1, k_2). \tag{2.31}$$

Finally, substitution of (2.31) into (2.28) leads to

$$A(k_1, k_2) = \beta(-k_1)\beta(-k_2)B(-k_1, k_2)\, e^{-ik_2} \tag{2.32}$$

where $B(k, k')$ is defined in (2.25).

2.3. *General n*

The above can be generalised to arbitrary values of n. The ansatz for the wavefunction becomes

$$f(x_1, \ldots, x_n) = \sum_P \varepsilon_P A(k_1, \ldots, k_n)\, e^{i(k_1 x_1 + \ldots + k_n x_n)} \tag{2.33}$$

where the sum extends over all permutations and negations of $k_1, \ldots, k_n$ and ε_P changes sign at each such 'mutation'. The coefficients in the wavefunction are given by

$$A(k_1, \ldots, k_n) = \prod_{j=1}^{n} \beta(-k_j) \prod_{1 \le j < l \le n} B(-k_j, k_l)\, e^{-ik_j} \tag{2.34}$$

where $B(k, k')$ is defined in (2.25) and (2.22). The parameters $k_1, \ldots, k_n$ satisfy

$$\frac{\alpha(k_j)\beta(k_j)}{\alpha(-k_j)\beta(-k_j)} = \prod_{\substack{l=1 \\ \neq j}}^{n} \frac{B(-k_j, k_l)}{B(k_j, k_l)} \qquad j = 1, \ldots, n. \tag{2.35}$$

with $\alpha(k)$ and $\beta(k)$ defined in (2.10). The eigenvalues E are given by

$$E = -\tfrac{1}{2}[(L-1)\Delta + p + p'] - 2\sum_{j=1}^{n} (\cos k_j - \Delta). \tag{2.36}$$

Returning to the Hamiltonian (1.1), the two cases of interest are $p = p' = 0$ and $p = -p' = i\alpha$ with $\Delta = -\cos\gamma$ and $\alpha = \sin\gamma$, $\gamma \in [0, \pi)$. For both cases the eigenenergies are given by

$$E = -\tfrac{1}{2}(L-1)\Delta - 2\sum_{j=1}^{n} (\cos k_j - \Delta). \tag{2.37}$$

Taking the logarithm of (2.35) (see, e.g., Baxter 1982), the parameters $k_j, j = 1, \ldots, n$ satisfy

$$(L+1)k_j = \pi l_j - \Theta(k_j, -k_j)) - \tfrac{1}{2}\sum_{\substack{l=1 \\ \neq j}}^{n} [\Theta(k_j, -k_l) + \Theta(k_j, k_l)] \tag{2.38}$$

for the Ashkin-Teller case ($\alpha = 0$) and

$$Lk_j = \pi l_j - \tfrac{1}{2}\sum_{\substack{l=1 \\ \neq j}}^{n} [\Theta(k_j, -k_l) + \Theta(k_j, k_l)] \tag{2.39}$$

for the Potts case ($\Delta^2 + \alpha^2 = 1$). The phase factor appearing in these equations is the same as that for the periodic case (Yang and Yang 1966), namely

$$\Theta(k, k') = 2\tan^{-1}\left(\frac{\Delta \sin(k-k')/2}{\cos(k+k')/2 - \Delta\cos(k-k')/2}\right). \tag{2.40}$$

From the numerical evidence (see below), the lowest state in a given sector is obtained by choosing the integers $l_j = j, j = 1, \ldots, n$, as earlier surmised by Gaudin (1971, 1983). We now proceed to evaluate the ground state energy per site in the limit $L \to \infty$.

2.4. Thermodynamic limit for $|\Delta| < 1$

Define

$$\varphi(a, b) = -i\ln\left(\frac{\sinh(b-a)/2}{\sinh(b+a)/2}\right). \tag{2.41}$$

Taking $\Delta = -\cos\gamma$, $\gamma \in (0, \pi)$ and setting

$$P = i\varphi(i\gamma, \ln(p - \Delta)) \tag{2.42a}$$

$$P' = i\varphi(i\gamma, \ln(p' - \Delta)) \tag{2.42b}$$

the transformation $k_j \to \varphi(\alpha_j, i\gamma)$ transforms (2.35) into

$$2L\varphi(\alpha_j, i\gamma) + \varphi(\alpha_j, P) + \varphi(\alpha_j, P') = 2\pi l_j + \sum_{\substack{l=1 \\ \neq j}}^{n} [\varphi(\alpha_j - \alpha_l, i2\gamma) + \varphi(\alpha_j + \alpha_l, i2\gamma)] \qquad j = 1, \ldots, n \tag{2.43}$$

with $l_j = j$ and $n = L/2$ for the ground state. Although the equations (2.43) are not in the usual difference form (Baxter 1982) it is interesting to observe that they still describe the extremum of a function χ of the n variables α_j (Yang and Yang 1966):

$$\chi(\alpha_1, \ldots, \alpha_n) = \sum_{j=1}^{n} [2L\psi(\alpha_j, i\gamma) + \psi(\alpha_j, P) + \psi(\alpha_j, P') - 2\pi l_j \alpha_j] - \sum_{1 \leq j < l \leq n} [\psi(\alpha_j - \alpha_l, i2\gamma) + \psi(\alpha_j + \alpha_l, i2\gamma)] \tag{2.44}$$

where the function ψ is defined by $\psi' = \varphi$.

For large L we assume that the α_j become evenly distributed in some fixed interval $(0, Q)$. Let the number of α_j lying between α and $\alpha + d\alpha$ be $L\rho(\alpha)\, d\alpha$. Taking the limit $L \to \infty$ and differentiating (2.43) with respect to α we then have

$$\pi\rho(\alpha) = \varphi'(\alpha, i\gamma) - \tfrac{1}{2}\int_0^Q \rho(\beta)[\varphi'(\alpha - \beta, i2\gamma) + \varphi'(\alpha + \beta, i2\gamma)]\, d\beta. \tag{2.45}$$

Since ρ and φ' are even functions (2.45) can be written as

$$\pi\rho(\alpha) = \varphi'(\alpha, i\gamma) - \tfrac{1}{2}\int_{-Q}^{Q} \rho(\beta)\varphi'(\alpha - \beta, i2\gamma)\, d\beta \tag{2.46}$$

where Q is determined by

$$\int_0^Q \rho(\alpha)\, d\alpha = n/L. \tag{2.47}$$

Setting $Q = \infty$ the density of zeros is thus

$$\rho(\alpha) = \frac{1}{2\gamma \cosh(\pi\alpha/2\gamma)} \tag{2.48}$$

(this is twice the density that is obtained for the periodic case). The energy per site in this limit is the same as for the periodic chain (Yang and Yang 1966)

$$e_\infty(\gamma) = \lim_{L\to\infty}(E/L) = \tfrac{1}{2}\cos\gamma - 2\int_0^\infty \rho(\alpha)[\cosh\varphi(\alpha, i\gamma) + \cos\gamma]\, d\alpha = \tfrac{1}{2}\cos\gamma - 2\sin^2\gamma \int_0^\infty \frac{dx}{\cosh(\pi x)[\cosh(2\gamma x) - \cos\gamma]} \tag{2.49}$$

with

$$e_\infty(0) = \tfrac{1}{2} - 2\ln 2. \tag{2.50}$$

3. Conformal anomaly and surface energy

Cardy (1984a) has derived a set of important relations involving surface exponents by conformally transforming a given statistical model in the half plane into a strip of size

M. In the case of the Hamiltonian formalism these relations can be stated as follows. To each surface exponent x_s of the infinite system (Binder 1983, Cardy 1987) there corresponds a set of states in the finite free boundary Hamiltonian on M sites with energies, at the bulk critical point, given by

$$E_s(M, r) = E_0(M) + \pi\zeta(x_s + r)/M + o(M^{-1}) \qquad r = 0, 1, 2, \ldots . \tag{3.1}$$

Here $E_0(M)$ is the ground state energy of the finite chain and ζ is a constant which is usually unity in the transfer matrix formalism but for Hamiltonians is model dependent (Alcaraz and Drugowich de Felício 1984, von Gehlen *et al* 1986). The conformal anomaly c of the appropriate conformal class of the bulk transition governs the dominant universal finite-size corrections in the ground state energy per site (Blöte *et al* 1986, Affleck 1986)

$$E_0(M)/M = e_\infty + \frac{f_\infty}{M} - \frac{\pi\zeta c}{24M^2} + o(M^{-2}) \tag{3.2}$$

where e_∞ and f_∞ are, respectively, the bulk limits of the ground state and surface energy per site.

The main numerical computations presented in this paper were achieved by solving equations (2.38) and (2.39). We obtained, in this way, several eigenenergies in the various sectors of (1.1) for chain size up to $L = 512$. These eigenenergies were then identified with the corresponding levels in the models (1.2) and (1.3) on $M = L/2$ sites. To make this comparison, the Bethe ansatz results for small L were compared with the results obtained by directly diagonalising (1.2) and (1.3) with the Lanczos method. (In the case of the q-state Potts model with $q \neq 2, 3, 4$ we simply assume that the corresponding states are the analytic continuation of those occurring in (1.2).) For the remainder of this paper we use the eigenenergies of models (1.2) and (1.3) calculated through (1.1) and the relations (3.1) and (3.2) in order to obtain the surface exponents and conformal anomaly of all three models.

Before applying (3.1) and (3.2), however, we need to identify the factor ζ for the models under consideration. This same factor occurs in the analogous relations for the periodic boundary condition case. From the large-L behaviour of the ground state energy of the periodic XXZ model (Hamer 1985, 1986) we identify for (1.1) the value

$$\zeta_{XXZ} = \pi \sin\gamma/\gamma. \tag{3.3}$$

Use of the relations between (1.1) and the Ashkin-Teller (1.2) and Potts (1.3) models (Alcaraz *et al* 1987a, b) then leads to

$$\zeta_{AT} = \pi \sin\gamma/2\gamma \qquad \zeta_q = \frac{\pi\sqrt{4-q}}{4\cos^{-1}(\sqrt{q}/2)} \qquad (q < 4) \qquad \zeta_4 = \pi/2. \tag{3.4}$$

It is gratifying to observe that the earlier numerical estimates (von Gehlen *et al* 1986, von Gehlen and Rittenberg 1986a, b, c, 1987) of ζ_{AT} and ζ_q are in good agreement with the exact values given in (3.4).

As typical examples of our numerical computations we show in table 1(a) the ground state energy per site for $M = 2^l$, $l = 2, 3, \ldots, 8$, of the Ashkin-Teller model with couplings $\lambda = -\sqrt{3}/2$, $-1/2$, $1/2$, $1/\sqrt{2}$, and $\sqrt{3}/2$. The corresponding results for a $2M$-site XXZ chain can be simply obtained by exploiting the equivalence between (1.1) and (1.2) (in particular, $\Delta = -\lambda$). In table 1(b) we similarly show the ground state energy per site of the q-state Potts model for $q = 2, 3, 3.414\ldots(4\cos^2(\pi/8))$, $3.618\ldots(4\cos^2(\pi/10))$ and 4.

Table 1. The ground state energy per site of the quantum (*a*) Ashkin-Teller chain and (*b*) q-state Potts chain. Exact values denoted by * are given by doubling (2.49). The extrapolated results (†) were obtained from the sequence $M = 4, 6, 8, \ldots, 60$ (see text).

(*a*)

M	$\lambda = -\sqrt{3}/2$	$\lambda = -\frac{1}{2}$	$\lambda = \frac{1}{2}$	$\lambda = 1/\sqrt{2}$	$\lambda = \sqrt{3}/2$
4	−0.898 391	−0.999 749	−1.421 625	−1.527 916	−1.613 182
8	−0.955 665	−1.047 739	−1.458 847	−1.565 672	−1.652 109
16	−0.984 695	−1.072 596	−1.478 866	−1.585 976	−1.673 022
32	−0.999 322	−1.085 256	−1.489 283	−1.596 544	−1.683 900
64	−1.006 662	−1.091 646	−1.494 602	−1.601 942	−1.689 456
128	−1.010 339	−1.094 856	−1.497 291	−1.604 672	−1.692 265
256	−1.012 179	−1.096 465	−1.498 643	−1.606 045	−1.693 677
e_∞^*	−1.014 020...	−1.098 076...	−1.5	−1.607 423...	−1.695 095...
$f_\infty^\dagger$	0.471 568	0.412 883	0.348 076	0.353 553	0.363 777
$c^\dagger$	0.999 99 (6)	0.999 99 (5)	1.000 0 (3)	1.000 0 (1)	1.00 (5)

(*b*)

M	$q = 2$	$q = 3$	$q = 3.414...$	$q = 3.618...$	$q = 4$
4	−1.459 958	−1.580 754	−1.626 304	−1.647 982	−1.687 466
8	−1.532 473	−1.636 076	−1.675 238	−1.693 900	−1.727 934
16	−1.569 617	−1.665 066	−1.701 131	−1.718 317	−1.749 664
32	−1.588 434	−1.679 942	−1.714 489	−1.730 948	−1.760 964
64	−1.597 906	−1.687 482	−1.721 281	−1.737 379	−1.766 733
128	−1.602 659	−1.691 279	−1.724 706	−1.740 626	−1.769 650
256	−1.605 040	−1.693 185	−1.726 427	−1.742 257	−1.771 116
e_∞^*	−1.607 423...	−1.695 095...	−1.728 152...	−1.743 893...	−1.772 588...
$f_\infty^\dagger$	0.610 502	0.489 637	0.442 487	0.419 717	0.377 649
$c^\dagger$	0.500 00 (1)	0.799 9 (2)	0.89 (3)	0.93 (5)	0.99 (2)
c	0.5	0.8	0.892 857...	0.933...	1.0

To compute the conformal anomaly from (3.2), we need first to estimate the (non-universal) surface energy f_∞. We have done this using Van den Broeck and Schwartz (1979) approximates to extrapolate the sequence

$$f_M = M(E_0(M) - e_\infty) \to f_\infty \tag{3.5}$$

with e_∞ being obtained from the exact result (2.49). The resulting estimates are quoted in table 1 and are believed to be accurate to the number of digits quoted. With f_∞ thus estimated, we can then estimate the conformal anomaly c by similarly extrapolating the sequence

$$c(M) \equiv -[E_0(M) - Me_\infty - f_\infty]24M/\pi\zeta. \tag{3.6}$$

The resulting estimates, again obtained by Van den Broeck and Schwartz approximates, are shown in table 1. From the table, we clearly see that $c = 1$, independent of Δ and λ, for the XXZ and Ashkin-Teller models which is expected due to their non-universal behaviour. We also see for the Potts chain that $c = \frac{1}{2}, \frac{4}{5}, \frac{25}{28}, \frac{14}{15}$ and 1 for the respective values of q. (The poorer convergence as q nears 4 is a result of the correction terms in (3.2) increasing with importance in this limit, in particular logarithmic corrections appear at $q = 4$ (Cardy 1986b, Woynarovich and Eckle 1987, Alcaraz *et al* 1987a, b).)

These values agree with the predicted values from conformal invariance (Dotsenko 1984, Cardy 1987). They are well accounted for by the expression (Alcaraz *et al* 1987a, b)

$$c(q) = 1 - \frac{6}{(\pi/\gamma)(\pi/\gamma - 1)} \qquad \gamma = \cos^{-1}\sqrt{q}/2. \tag{3.7}$$

The Bethe ansatz equations (2.39) decouple at the value $\gamma = \pi/2$ corresponding to the $q = 0$ limit. This limit further corresponds to the Hamiltonian analogue of a resistor network (see, e.g., Wu 1982). From (2.37) the ground state energy per site is exactly given by

$$E_0/M = -2\sqrt{2}\cos\frac{\pi}{4}\left(1+\frac{1}{M}\right)\operatorname{cosec}\frac{\pi}{4M} \tag{3.8}$$

which on expressing in powers of $1/M$ and comparing with (3.2) yields the exact values $f_\infty = 1$ and $c = -2$. In the $q = 1$ limit (percolation) we have $\gamma = \pi/3$ and although we are unable to solve (2.39) analytically our numerical results are reproduced for all M by

$$E_0/M = -\tfrac{3}{2}(1 - 1/2M) \tag{3.9}$$

which gives $e_\infty = -\frac{3}{2}$, $f_\infty = \frac{3}{4}$ and $c = 0$. It is interesting to observe that these results also fit the formula (3.7). This equation can be expressed in the standard form (see, e.g., Cardy 1987) by identifying $\pi/\gamma = m + 1$. We see that $c = -2$ and $c = 0$ respectively correspond to the values $m = 1$ and $m = 2$.

4. Surface exponents

We now turn to the surface exponents of the models under consideration. Let us consider initially an L-site XXZ model with free boundaries (equation (1.1) with $\alpha = 0$). It is convenient here to label the sectors by the number n, defined by $n = L/2 - n$, representing the number of over-turned spins from the antiferromagnetic ground state ($n = L/2$). Associated with the lowest energy $E_0^{(n)}$ in each sector we have a surface exponent $x_s^{(n)}$, which may be estimated from the sequence (recall (3.1))

$$x_s^{(n)}(L) \equiv [E_0^{(n)} - E_0^{(0)}]\frac{L}{\pi\zeta} \qquad n = 1, 2, \ldots \tag{4.1}$$

where $E_0^{(0)}$ is the ground state energy and ζ is given in (3.3). For $n = 1, 2, \ldots$ these dimensions govern, respectively, the decay of the spin-spin, energy-energy, ... correlations. In table 2 we show, for several values of $\lambda = -\Delta$, the extrapolated values of the above sequence. Our results strongly suggest that these exponents are given by

$$x_s^{(n)} = 2n^2 x_p \qquad n = 1, 2, \ldots \tag{4.2}$$

where $x_p \equiv (\pi - \gamma)/2\pi$ is the anomalous dimension of the bulk polarisation operator. In comparison, the corresponding scaling dimensions for the bulk correlation functions are given by $x^{(n)} = n^2 x_p$, $n = 1, 2, \ldots$ (Alcaraz *et al* 1987a, b).

For the case of the Ashkin-Teller chain the Hamiltonian (1.2) is invariant under $Z(2) \otimes Z(2)$ internal symmetry as well as possessing reflection symmetry. The Hilbert space decomposes into eight sectors with corresponding energies $E_r^{(Q,P)}$ where $Q = 0, 1, 2, 3$, $P = \pm$ and $r = 0, 1, 2, \ldots$. The sectors with $Q = 1$ and $Q = 3$ are degenerate

Table 2. Extrapolated and expected results for the leading surface exponents of the *XXZ* and Ashkin-Teller chains.

λ	$x_s^{(1)} \equiv x_s^{(1,+)}$	$x_s^{(2)}$	$x_s^{(3)}$	$x_s^{(1,-)}$	$x_s^{(2,+)}$	$x_s^{(2,-)}$
$-\sqrt{3}/2$	0.166 666 (9) ($\frac{1}{6}$)	0.666 666 (5) ($\frac{2}{3}$)	1.500 00 (3) ($\frac{3}{2}$)	1.16 (4) ($\frac{7}{6}$)	—	—
$-\frac{1}{2}$	0.333 333 (3) ($\frac{1}{3}$)	1.333 33 (8) ($\frac{4}{3}$)	3.000 0 (1) (3)	1.333 33 (5) ($\frac{4}{3}$)	1.000 00 (6) (1)	2.000 00 (4) (2)
$\frac{1}{2}$	0.666 6 (7) ($\frac{2}{3}$)	2.666 (8) ($\frac{8}{3}$)	6.000 (2) (6)	1.666 6 (5) ($\frac{5}{3}$)	1.000 0 (7) (1)	2.000 (2) (2)
$1/\sqrt{2}$	0.750 00 (7) ($\frac{3}{4}$)	2.999 9 (3) (3)	6.749 (7) ($\frac{27}{4}$)	1.750 0 (4) ($\frac{7}{4}$)	1.000 0 (4) (1)	1.999 9 (9) (2)

due to the global symmetry $\sigma \Leftrightarrow \tau$ in (1.2). In each of these sectors we identify the corresponding surface exponent $x_s^{(Q,P)}$ from the sequence

$$x_s^{(Q,P)}(M) \equiv [E_0^{(Q,P)} - E_0^{(0,0)}] \frac{M}{\pi\zeta} \qquad Q = 1, 2, 3 \qquad P = \pm \tag{4.3}$$

with ζ given by (3.4). These sequences are listed in table 3 for the particular value $\lambda = \frac{1}{2}$ and chain sizes $M = 2^l$ for $l = 2, 3, \ldots, 8$. Extrapolated results for several λ values are given in table 2. We observe from these results that $x_s^{(Q,-)} = x_s^{(Q,+)} + 1$, implying that for a given charge Q, the ground state in the positive (negative) parity sector corresponds to the first (second) state in the tower of states given in (3.1). In agreement with earlier numerical results (von Gehlen and Rittenberg 1986c, 1987), our results clearly show that the surface exponents describing the magnetic and electric correlations $x_s^m = \eta_\parallel^{m/2}$ and $x_s^e = \eta_\parallel^e/2$, respectively, are given by

$$x_s^m \equiv x_s^{(1,+)}(\infty) = (\pi - \gamma)/\pi = (2x_\varepsilon^{AT})^{-1} \qquad \text{for} \qquad -1 \leq \lambda \leq 1 \tag{4.4}$$

$$x_s^e \equiv x_s^{(2,+)}(\infty) = 1 \qquad \text{for} \qquad -1/\sqrt{2} \leq \lambda \leq 1 \tag{4.5}$$

where x_ε^{AT} is the anomalous dimension of the energy operator. The levels $E_0^{(2,+)}$ and $E_0^{(2,-)}$ are both in the $n = 0$ ($n = M$) sector of (1.1) with $L = 2M$ and the integers l_j chosen from $\{1, 2, \ldots, n-1, n+1\}$ and $\{1, 2, \ldots, n-2, n, n+1\}$, respectively. For both the Ashkin-Teller and Potts models (see below) the levels $E_0^{(1,+)}$ and $E_0^{(1,-)}$ occur in the $n = 1$ ($n = M - 1$) sector of (1.1) again with $L = 2M$ but with respective integer sets $\{1, 2, \ldots, n\}$ and $\{1, 2, \ldots, n-1, n+1\}$. Unfortunately, due to numerical

Table 3. Amplitude estimates (4.3) for the Ashkin-Teller chain at $\lambda = \frac{1}{2}$.

M	$x_s^{(1,+)}(M)$	$x_s^{(1,-)}(M)$	$x_s^{(2,+)}(M)$	$x_s^{(2,-)}(M)$
4	0.547 542	1.345 31	0.777 955	1.555 91
8	0.596 800	1.496 16	0.880 264	1.760 53
16	0.626 720	1.574 75	0.935 469	1.870 94
32	0.644 236	1.616 43	0.965 016	1.930 03
64	0.654 243	1.639 07	0.980 990	1.961 98
128	0.659 859	1.651 54	0.989 687	1.979 37
256	0.662 969	1.658 41	0.994 425	1.988 85
Exact	$\frac{2}{3}$	$\frac{5}{3}$	1	2

instabilities we are unable to compute the level in (1.1) corresponding to x_s^e inside the critical fan region ($-1 \leqslant \lambda \leqslant -1/\sqrt{2}$).

In the case of the q-state Potts model ($q \in Z$) the Hamiltonian (1.3) is symmetric under global $Z(q)$ transformations and reflections of the lattice. Consequently the Hilbert space separates into $2q$ disjoint sectors with energies $E_r^{(Q,P)}$ ($Q = 0, 1, \ldots, q-1$, $P = \pm$, $r = 0, 1, 2, \ldots$). The ground state lies in the sector labelled by $Q = 0$, $P = +$, ($r = 0$) while the sectors with $Q \neq 0$ are degenerate. In this case the leading surface exponent can be extracted by extrapolating the estimators (4.3) with $Q = 1$ and the corresponding ζ given in (3.4). In table 4 we show the sequence $x_s^{(1,+)}(L)$ with $M = 2^l$, $l = 2, 3, \ldots, 8$ for $q = 1, 2, 3, 3.414\ldots(4\cos^2(\pi/8)), 3.618\ldots(4\cos^2(\pi/10))$ and 4. As in the Ashkin-Teller case we have also verified that $x_s^{(1,-)} = x_s^{(1,+)} + 1$ which as before implies that the lowest state in the negative parity sector corresponds to the second level in the tower of states characterising $x_s = \eta_\parallel/2 \equiv x_s^{(1,+)}(\infty)$. All of the observed values are well accounted for by the expression

$$x_s = 1 - 2\gamma/\pi \qquad q = 4\cos^2\gamma \tag{4.6}$$

which agrees with the predicted value (Cardy 1984b) $x_s = (m-1)/(m+1)$, $m = 1, 2, 3, 5, \ldots$ if we again identify $\pi/\gamma = m+1$. In the limit $q = 0$, corresponding to $m = 1$, the Bethe ansatz equation (2.39) and (2.37) yield the exact equality $E_0^{(0,+)}(M) = E_0^{(1,+)}(M)$ giving $x_s = \eta_\parallel = 0$ in agreement with (4.6). Again the convergence of the sequences deteriorates as we approach the limit $q = 4$ where the logarithmic corrections occur. The extrapolated value for $q = 4$ quoted in table 4 is obtained by assuming a logarithmic correction in (4.3) of the form predicted by Cardy (1986b).

Table 4. Amplitude estimates (4.3), $x_s^{(1,+)}(M)$, for the q-state Potts chain.

M	$q=1$	$q=2$	$q=3$	$q=3.414\ldots$	$q=3.618\ldots$	$q=4$
4	0.310 468	0.442 191	0.546 487	0.585 170	0.603 466	0.636 608
8	0.322 203	0.469 919	0.595 135	0.643 906	0.667 460	0.710 956
16	0.327 900	0.484 665	0.624 763	0.681 940	0.710 179	0.763 490
32	0.330 662	0.492 260	0.642 322	0.706 203	0.738 489	0.800 955
64	0.332 012	0.496 112	0.652 588	0.721 662	0.757 377	0.828 331
128	0.332 677	0.498 051	0.658 548	0.731 552	0.770 131	0.848 934
256	0.333 006	0.499 025	0.661 992	0.737 920	0.778 858	0.864 907
Extrapolated	0.333 33 (3)	0.500 00 (0)	0.666 66 (9)	0.749 (8)	0.799 (6)	0.99 (3)
Exact	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{2}{3}$	$\frac{3}{4}$	$\frac{4}{5}$	1

Acknowledgments

It is a pleasure to acknowledge profitable discussions with Dr C J Hamer. This work was supported in part by the Australian Research Grant Scheme, the Commonwealth Department of Education through a Commonwealth Postgraduate Research Award and by Fundacão de Amparo à Pesquisa do Estado de São Paulo, Brasil.

Note added in proof. After submitting this paper the conformal anomaly and surface energy of the Potts and Ashkin-Teller chains were derived exactly by Hamer *et al* (1987).

References

Affleck I 1986 *Phys. Rev. Lett.* **56** 746

Alcaraz F C, Barber M N and Batchelor M T 1987a *Phys. Rev. Lett.* **58** 771

—— 1987b to be published

Alcaraz F C and Drugowich de Felício J R 1984 *J. Phys. A: Math. Gen.* **17** L651

Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (New York: Academic)

Belavin A A, Polyakov A M and Zamolodchikov A B 1984 *Nucl. Phys.* B **241** 333

Binder K 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic) p 1

Blöte H W J, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742

Cardy J L 1984a *J. Phys. A: Math. Gen.* **17** L385

—— 1984b *Nucl. Phys.* B **240** [FS12] 514

—— 1986a *Nucl. Phys.* B **270** [FS16] 186

—— 1986b *J. Phys. A: Math. Gen.* **19** L1093

—— 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55

Dotsenko Vl S 1984 *Nucl. Phys.* B **235** 54

Gaudin M 1971 *Phys. Rev.* A **4** 386

—— 1983 *La Fonction d'Onde de Bethe* (Paris: Masson)

Hamer C J 1981 *J. Phys. A: Math. Gen.* **14** 2981

—— 1985 *J. Phys. A: Math. Gen.* **18** L1133

—— 1986 *J. Phys. A: Math. Gen.* **19** 3335

Hamer C J, Quispel G R W and Batchelor M T 1987 *J. Phys. A: Math. Gen.* **20** 5677

Kohmoto M, den Nijs M and Kadanoff L P 1981 *Phys. Rev.* B **24** 5229

Polyakov A M 1970 *Zh. Eksp. Teor. Fiz. Pis. Red.* **12** 538 (1970 *JETP Lett.* **12** 381)

Van den Broeck J-M and Schwartz L W 1979 *SIAM J. Math. Anal.* **10** 658

von Gehlen G and Rittenberg V 1986a *J. Phys. A: Math. Gen.* **19** L625

—— 1986b *J. Phys. A: Math. Gen.* **19** L631

—— 1986c *J. Phys. A: Math. Gen.* **19** L1039

—— 1987 *J. Phys. A: Math. Gen.* **20** 227

von Gehlen G, Rittenberg V and Ruegg H 1986 *J. Phys. A: Math. Gen.* **19** 107

Woynarovich F and Eckle H-P 1987 *J. Phys. A: Math. Gen.* **20** L97

Wu F 1982 *Rev. Mod. Phys.* **54** 235

Yang C N and Yang C P 1966 *Phys. Rev.* **150** 321, 327