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The spin- S XXZ quantum chain with general toroidal boundary conditions

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Abstract. We derive the operator content of the spin- S XXZ quantum chain with generalised toroidal boundary conditions compatible with the $U(1)$ symmetry of the model. These results are derived by solving numerically the associated Bethe ansatz equations for finite chains and exploring the consequences of the conformal invariance of the infinite system. We also show that, as in the spin- $\frac{1}{2}$ case, the conformal anomaly and dimensions of general extended $SU(2)$ algebras can be obtained from these spin- S chains by choosing properly the coupling constant and the boundary condition.

1. Introduction

In two dimensions the conformal invariance at the critical point of the statistical systems powerfully constrains the possible universality classes of critical behaviour [1, 2]. These universality classes are labelled by the dimensionless number c , which is the central charge or conformal anomaly of the associated Virasoro algebra. In the case where $c < 1$ the requirement of reflection positivity (unitarity) of the transfer matrix [2] restricts c to the countable set

$$c = 1 - \frac{6}{m(m+1)} \quad m = 3, 4, 5, \dots \quad (1.1)$$

In this minimal series, which includes the Ising ($m = 3$), the three-state Potts model ($m = 5$), the algebra is finite and the scaling dimensions $(\Delta_{p,q}, \bar{\Delta}_{p,q})$ are given by the Kac formula

$$\Delta_{p,q} = \frac{[p(m+1) - qm]^2 - 1}{4m(m+1)} \quad 1 \leq p \leq m-1, 1 \leq q \leq m. \quad (1.2)$$

When $c \geq 1$ the algebra is not finite and unitarity does not restrict the values of c . These values are again constrained when the primary fields obey an extended algebra, larger than the Virasoro algebra. These are the cases of models exhibiting supersymmetry [3] where

$$c = \frac{3}{2} \left(1 - \frac{8}{m(m+2)} \right) \quad m = 3, 4, \dots \quad (1.3)$$

$Z(N)$ is the Zamolodchikov-Fateev parafermionic algebra [4] where

$$c = \frac{2(N-1)}{N+2} \quad N = 2, 3, 4, \dots \quad (1.4)$$

and the Kac-Moody algebra, where c is a function of the topological charge k and the associated semisimple group G , in the case where G is the $SU(2)$ group [5], is

$$c = \frac{3k}{1+k}. \quad (1.5)$$

More generally, it was shown [6] using a Feigin-Fuchs construction [7] that a general set of theories can be derived from those described by the $SU(2)$ Kac-Moody algebra with topological charge k . The conformal anomaly of these theories is given by

$$c = \frac{3k}{k+2} \left(1 - \frac{2(k+2)}{m(m+k)} \right) \quad m = 3, 4, \dots; k = 1, 2, \dots \quad (1.6)$$

and the corresponding scaling dimensions ($\Delta_{p,q}$, $\bar{\Delta}_{p,q}$) are given by a generalisation of the Kac formula (1.2)

$$\Delta_{p,q} = \frac{[p(m+k) - qm]^2 - k^2}{4km(m+k)} + \frac{t(k-t)}{2k(k+2)} \quad (1.7a)$$

where

$$m = 3, 4, \dots; 1 \leq p \leq m-1; 1 \leq q \leq m+k-1; t = (p-q) \bmod 2k; 0 \leq t \leq k. \quad (1.7b)$$

The cases $k=1$ and $k=2$ recover the minimal and supersymmetric series given by (1.1) and (1.3) respectively. As $m \rightarrow \infty$ we obtain the conformal anomaly of a $SU(2)$ Kac-Moody algebra with topological charge k .

In a previous paper [8] we have obtained the operator content of a special set of antiferromagnetic quantum Hamiltonians defined on a periodic chain. These Hamiltonians describe the dynamics of particles with arbitrary spin ($S = 1, \frac{3}{2}, 2, \dots$) and are generalisations of the standard $S = \frac{1}{2}$ anisotropic Heisenberg model or XXZ quantum chain. These spin chains are exactly integrable through the Bethe ansatz. Analysing numerically their eigenspectrum, with periodic boundaries, we verified [8] that they are described by a $c = 3S/(1+S)$ conformal field theory, described in terms of composite field operators formed by the product of Gaussian fields ($c=1$) and $Z(2S)$ Zamolodchikov-Fateev operators ($c = (2S-1)/S+1$). These spin chains also correspond to a generalised Coulomb gas [9].

In the case of the $S = \frac{1}{2}$ XXZ chain ($c = \frac{1}{2}$) it was shown [10, 11] that the operator content of other models with $c < 1$ can be obtained by changing continuously the boundary conditions. This fact motivated us to study the operator content of the general spin- S XXZ chain ($c = 3S/(1+S)$) with generalised toroidal boundary conditions, in order to see if we can recover the conformal anomaly and dimensions of the $c < 3S/(1+S)$ theories.

The operator content for these spin chains will be calculated by exploiting the relationship [12] between the eigenspectrum of the finite chain (size L), at the critical point, and the conformal anomaly and scaling dimensions of the operators governing the critical behaviour. The conformal anomaly c can be derived from the finite-size corrections of the ground state $E_0(L)$ of the finite chain [13]. For periodic boundaries

$$\frac{E_0(L)}{L} = e_\infty - \frac{\pi c \zeta}{6L^2} + o(L^{-2}) \quad (1.8)$$

where e_∞ is the bulk limit of the ground-state energy and ζ is the sound velocity. On the other hand the scaling dimensions of the primary operators can be evaluated from

the finite-size corrections of the excited states. For each primary operator $\psi_{\Delta, \bar{\Delta}}$, with dimensions $X = \Delta + \bar{\Delta}$ and spin $s = \Delta - \bar{\Delta}$ there exists a tower of states in the finite L chain. The energy and momentum of these states are given by [12]

$$E_{M, \bar{M}} = E_0(L) + 2\pi\zeta(X + M + \bar{M})/L + o(L^{-1}) \tag{1.9a}$$

$$P_{M, \bar{M}} = \frac{2\pi}{L}(s + M - \bar{M}) \quad M, \bar{M} = 0, 1, 2, \dots \tag{1.9b}$$

The layout of this paper is as follows. In section 2 we present the models and their associated Bethe ansatz equations, for the case of general toroidal boundary conditions. These equations are analysed numerically in sections 3 and 4. In section 3 we present some distributions of zeros of these equations and in section 4 the operator content of the spin- S XXZ model with general toroidal boundaries is derived. Finally in section 5 we show that the dimensions (1.7) of the extended algebras (1.6) can be obtained from the operator content derived in section 4.

2. The Bethe ansatz and the spin- S XXZ chain with general toroidal boundary conditions

The spin- $S = \frac{1}{2}$ XXZ chain with anisotropy constant γ and Hamiltonian

$$H_{XXZ}^{(1/2)}(\gamma) = -\frac{1}{2} \sum_{i=1}^L (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y - \cos \gamma \sigma_i^z \sigma_{i+1}^z) \tag{2.1}$$

describes the dynamic of spin- $S = \frac{1}{2}$ Pauli matrices ($\sigma_i^x, \sigma_i^y, \sigma_i^z$) located at the sites ($i = 1, 2, \dots, L$) of an L -site chain. The exact solution of the eigenenergies of (2.1) in a periodic chain, is one of most known examples of the success of the Bethe ansatz technique.

The generalisation of (2.1), for a spin- $S = 1$ model, preserving integrability is given by the Hamiltonian [15]

$$H_{XXZ}^{(1)}(\gamma) = \frac{1}{4} \sum_{i=1}^L \{ \sigma_i - (\sigma_i)^2 - 2(\cos \gamma - 1)(\sigma_i^+ \sigma_i^- + \sigma_i^- \sigma_i^+) - 2 \sin^2 \gamma (\sigma_i^z - (\sigma_i^z)^2 + 2(S_i^z)^2 - 2) \} \tag{2.2a}$$

where

$$\sigma_i = S_i S_{i+1} = \sigma_i^+ + \sigma_i^-; \quad \sigma_i^z = S_i^z S_{i+1}^z \tag{2.2b}$$

and S^x, S^y and S^z are the (3×3) SU(2)-matrices of spin-1. The generalisation to arbitrary spin- S [16] is a polynomial of degree $2S$ in the variables σ_i^+, σ_i^- and S_i^z . The isotropic limit ($\gamma = 0$) of these models corresponds to the spin- S Takhtajan-Babudjian Hamiltonian [17]. These antiferromagnetic spin- S chains are massless for $0 \leq \gamma \leq \pi$ and in previous publications [8] we have calculated their operator content for $0 \leq \gamma \leq \pi/2S$ and periodic boundary conditions. In this paper we will calculate the operator content for these quantum chains with the boundary condition ($0 \leq \phi < \pi$):

$$S_{L+1}^\pm = S_{L+1}^x \pm i S_{L+1}^y = e^{\pm i\phi} (S_1^x \pm i S_1^y) \quad S_{L+1}^z = S_1^z \tag{2.3}$$

which corresponds to a rotation by an angle ϕ of the last spin around the z axis. These spin- S quantum chains, in the periodic case, are related to $(2S + 1)$ colour-vertex

models defined in a torus with a perimeter L in one direction and an infinite perimeter in the other direction (time). The boundary conditions (2.3) correspond to the introduction of a seam with different Boltzmann weights along the time direction. In the spin- $S = \frac{1}{2}$ case ($c = 1$) the effect of these boundaries [10, 11] in the Hamiltonian, or the seam line in the vertex models [18], is the reduction of the finite-size corrections, producing the same corrections as a $c < 1$ theory in a periodic chain.

The spin- S quantum chain has in general a $U(1)$ symmetry corresponding to the commutation of the total spin operator

$$\hat{S}^z = \sum_{i=1}^L S_i^z.$$

The boundary condition (2.3) is the most general boundary condition compatible with this $U(1)$ symmetry and consequently we can, as in the periodic case ($\phi = 0$), separate the Hilbert space in disjoint sectors labelled by the eigenvalues of \hat{S}^z , namely $n = 0, \pm 1, \pm 2, \dots, \pm LS$ for L even and for L odd $n = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots, \pm LS$ ($n = 0, \pm 1, \pm 2, \dots, \pm LS$) if S is half-integer (integer).

The Bethe ansatz equations, for the periodic case, were derived by Sogo [16]. We present now the corresponding equations for the case of the boundary conditions (2.3). The eigenenergies, for a given sector n , are given in terms of the $(SL - n)$ complex roots $(\lambda_1, \lambda_2, \dots, \lambda_{SL-n})$ of the nonlinear set of Bethe ansatz equations (BAE)

$$e^{i\phi} \left\{ \frac{\sinh \gamma(\lambda_j - iS)}{\sinh \gamma(\lambda_j + iS)} \right\}^L = - \prod_{k=1}^{SL-n} \frac{\sinh \gamma(\lambda_j - \lambda_k - i)}{\sinh \gamma(\lambda_j - \lambda_k + i)} \quad j = 1, 2, \dots, SL - n. \tag{2.4}$$

The eigenenergies are given by

$$E = \frac{\sin^2(2S\gamma)}{2S} \sum_{j=1}^{SL-n} \frac{1}{\cos 2S\gamma - \cosh 2\lambda_j}. \tag{2.5}$$

The above equations recover the periodic case [16], when $\phi = 0$, for general S as well the spin- $S = \frac{1}{2}$ case with arbitrary angle ϕ [10].

3. Numerical solutions of the Bethe ansatz equations

In [8] and [10] we can find an extensive list of previous works based on the solution of the BAE for finite systems. In [8] we have analysed extensively equation (2.4) in the periodic case ($\phi = 0$) and in this section we will report our results for the general angle ϕ in the region where $0 \leq \gamma \leq \pi/2S$. The equations for $\phi \neq 0$ are in general more difficult to solve numerically because in this case, contrary to the periodic case [8], we should always search for non-symmetric distribution of zeros with respect to the imaginary axes. This is due to the fact that in the case where $\phi \neq 0$ even the zero-momentum states have non-symmetrical distribution of zeros. Because of this most of our numerical analysis will be done for the spin- $S = 1$ system.

We solve the BAE (2.4) by using the Newton-type method for systems of size $L = 2-40$. We can easily extend these lattice chains up to $L \sim 100$, which is not necessary for our purposes. We solve initially the simplest case where $\phi = 0$ and we use this solution as an initial guess for the $\phi \neq 0$ system.

In order to proceed let us now discuss briefly how to implement a vectorial basis, with momentum quantum numbers, for the general toroidal boundary conditions (2.3).

For simplicity, assume we are using the basis in which S^z is diagonal, i.e.

$$S_j^z |s_1, s_2, \dots, s_j, \dots, s_L\rangle = s_j |s_1, s_2, \dots, s_L\rangle \tag{3.1}$$

where $s_j = -S, -S+1, \dots, S$. In this case the Hilbert space is already separated in block disjoint sectors labelled by

$$n = \sum_{i=1}^L S_i^z.$$

The momentum states in a given sector n , are given by the states with positive norm

$$\begin{aligned} \psi_{k+\phi_n/2\pi} = \frac{1}{\sqrt{L}} \{ & |s_1, s_2, \dots, s_L\rangle + C_1 |s_L, s_1, s_2, \dots, s_{L-1}\rangle \\ & + C_2 |s_{L-1}, s_L, s_1, \dots, s_{L-2}\rangle + \dots + C_{L-1} |s_2, s_3, \dots, s_L, s_1\rangle \} \end{aligned} \tag{3.2a}$$

where

$$C_t = \exp\left[i t \frac{2\pi}{L} \left(k - \frac{\phi n}{2\pi} \right) \right] \exp\left(i \phi \sum_{j=0}^{t-1} s_{L-j} \right) \quad k, t = 0, 1, 2, \dots, L-1. \tag{3.2b}$$

We therefore see that for the general toroidal boundary conditions (2.3), the momentum numbers will depend on the boundary angle ϕ and the particular sector n . In units of $2\pi/L$ they are given by

$$P = k - \frac{\phi n}{2\pi} \quad k = 0, 1, 2, \dots, L-1. \tag{3.3}$$

3.1. Lowest-energy state in sector n

Our numerical results indicate that the ground state occurs in the sector $n = 0$, being a zero momentum state ($k = 0$ in 3.3). Although the state has no momentum the distribution of zeros is not symmetrical with respect to the imaginary axis. The roots $\{\lambda_j, j = 1, \dots, LS\}$, independently of the values of γ ($0 \leq \gamma\pi/2S$), cluster in a sea of $L/2$ string-like complexes of size $2S$, where the imaginary parts are approximately equally spaced. These results are in accordance with the string hypothesis, which asserts that as $L \rightarrow \infty$ these complexes become strings of size $2S$. In figure 1 we show the distribution of λ in the complex plane for the spin- $S = 1$ and $S = \frac{3}{2}$ model in a $L = 8$ lattice, with coupling $\gamma = \pi/5$ and boundary angle $\phi = \pi/5$. Like in the periodic case [8, 16], as l increases the distribution of zeros tends towards a sea of $L/2$ strings of size $2S$.

The lowest energy states in the other sectors ($n \neq 0$) are non-zero momentum states ($k \neq 0$ in 3.3). The string assumption [16] when applied to the BAE (2.4) asserts that the roots, as $L \rightarrow \infty$, cluster into $(L/2 - 1 - [n/2S])$ string-like structures of size $2S$ and one string-like structure of size $(2S - \{n/2S\})$, where we define $[a/b]$ and $\{a/b\}$ as the integer-part and the rest of the ratio a/b , respectively. Our numerical results for the spin $S = 1$ case are in agreement with this hypothesis, and in figure (2d) and figure (2f) we show, for the $L = 4$ spin-1 chain these configurations in the sectors $n = 1$ and $n = 2$, respectively. However, as in the periodic case [8], for $S \geq \frac{3}{2}$ our numerical investigations also show violations in the above string assumption.

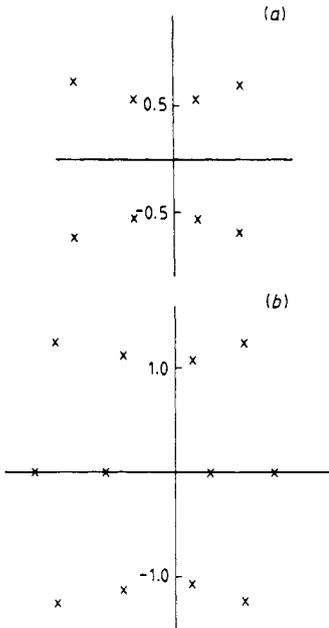


Figure 1. Typical distribution of zeros of the Bethe ansatz equations for the ground state of the spin- S XXZ chain with coupling $\gamma = \pi/5$ and boundary angle $\phi = \pi/5$. The vertical (horizontal) axis represents the imaginary (real) part of the roots. (a) spin- $S=1$, (b) spin- $S=3/2$.

3.2. Excited states

In figure 2 we show schematically for spin-1 in an $L=4$ chain, the distribution of zeros corresponding to some excited states. For larger lattices we only have to add strings of size $2S$ in the configurations of figure 2. Figures 2(b) and 2(c) are excited states in the sector $n=0$ while figures 2(e) and 2(g) are excited states in the sectors $n=1$ and $n=2$, respectively. The zeros denoted by asterisks (antiparticles) have an imaginary part exactly given by $\pi/2\gamma$ and those by circles are real numbers. Other types of excitations, involving strings of size greater than two, are very difficult to obtain due to numerical instabilities.

4. Finite-size corrections and the operator content of the spin- S XXZ chain

We will investigate in this section the operator content of the spin- S XXZ chain. Our numerical results show that for a fixed value of the lattice size L and the anisotropy γ , the ground-state energy $E_0^{(0)}(\gamma, L, \phi)$ has a minimum for $\phi=0$ (periodic). From this fact we may consider the eigenstates of the spin chain with toroidal boundary condition (2.3), specified by the angle $\phi \neq 0$, as excitations above the true ground-state energy $E_0^{(0)}(\gamma, L, 0)$. From (1.9) the scaling dimensions of the operators related to

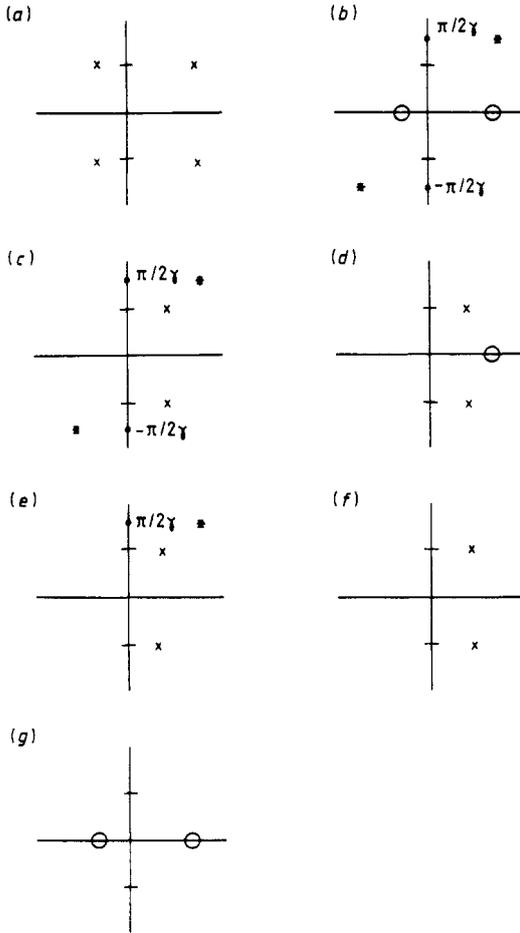


Figure 2. Some typical configuration of the complex zeros of the Bethe ansatz equations for the spin-1 XXZ Hamiltonian, with boundary angle $\phi \neq 0$ in an $L = 4$ chain. The vertical (horizontal) axis represents the imaginary (real) part of the roots. The zeros forming string-like excitations of size 2 are represented by crosses (x), the real zeros by circles (o) and the zeros with imaginary part exactly given by $\pm\pi/2\gamma$ are represented by asterisks (*). Figures (a), (b) and (c) represent states in the sector $n = 0$, figures (d) and (e) states in the sector $n = 1$ and figure (f) and (g) states in the $n = 2$ sector. Figures (a), (d) and (f) correspond to the lowest-energy state of sectors $n = 0, 1$ and 2 , respectively.

these excitations can be calculated by extrapolating the sequences

$$\Lambda_n^{(r)}(\gamma, L, \phi) = \frac{L}{2\pi\zeta} [E_n^{(r)}(\gamma, L, \phi) - E_0^{(0)}(\gamma, L, 0)] \quad (4.1)$$

where $E_n^{(r)}(\gamma, L, \phi)$ is the r th excited eigenstate in the sector n of the quantum chain with toroidal boundary condition specified by ϕ . In (4.1) the constant ζ is the sound velocity, which does not depend on the particular boundary condition we choose and consequently, from the results of the periodic case [8, 16]

$$\zeta = \pi \frac{(\sin 2S\gamma)}{4\gamma} \quad 0 \leq \gamma \leq \pi/2. \quad (4.2)$$

In table 1 we show the extrapolated results $\Lambda_n^{(0)}(\gamma, \infty, \phi)$ for some values of γ and ϕ for the spin- $S = 1$ and spin- $S = \frac{3}{2}$ chains. The extrapolated results $\Lambda_0(\gamma, \infty, \phi)$ of these sequences give us the scaling dimension

$$X_{0,\phi S/\pi}^{(S)} = (\phi S/\pi)^2 / (4S)^2 X_p^{(S)} \tag{4.3}$$

where

$$X_p^{(S)} = \frac{(\pi - 2S\gamma)}{4\pi S}. \tag{4.4}$$

These conjectured values are also shown in table 1.

Let us restrict, for the moment, with the spin- $S = 1$ chain where most of our numerical analysis was done. The extrapolated values of the finite-size sequences $\Lambda_n^{(0)}(\gamma, L, \phi)$, associated to the lowest-energy state in the sector $n \neq 0$, give us the scaling dimensions

$$X_{n,\phi/\pi}^{(1)} = n^2 X_p^{(1)} + \frac{(\phi/\pi)^2}{4^2 X_p^{(1)}} + \frac{t}{8} \quad t = n \bmod 2 \tag{4.5}$$

where $X_p^{(1)}$ is given by (4.4). It is interesting to observe here that, from our analysis of section 3, the lowest state in a given sector n has momentum $n\phi/2\pi$. Consequently if (4.5) is related to the dimensions of a primary operator ($M = \bar{M} = 0$ in 1.9) its spin should be $n\phi/2\pi$, which means that the operator is not scalar unless $n = 0$.

From the results of the periodic case [8] as well from the results of the spin- $\frac{1}{2}$ chain with boundary angle ϕ [10] we are induced to interpret the dimensions (4.3) and (4.4) as arising from composite operators

$$\psi_{\Delta_I, \bar{\Delta}_I}^{n,m+\phi/\pi} = \sigma_{\Delta_I, \bar{\Delta}_I} \phi_{\Delta_+^{(1)}, \Delta_-^{(1)}}^{n,m+\phi/\pi} \tag{4.6a}$$

formed by the product of Ising operators $\sigma_{\Delta_I, \bar{\Delta}_I}$ with dimensions $(\Delta_I, \bar{\Delta}_I)$ and a Gaussian-type operator $\phi_{\Delta_+^{(1)}, \Delta_-^{(1)}}^{n,m+\phi/\pi}$ with dimensions $(\Delta_+^{(1)}, \Delta_-^{(1)})$, describing an excitation with spin wavenumber n and vorticity $(m + \phi/\pi)$ where

$$\Delta_I, \bar{\Delta}_I = 0, 1/2, 1/16 \tag{4.6b}$$

$$\Delta_{\pm}^{(1)}(\phi) = \frac{1}{2} \left[n\sqrt{X_p^{(1)}} \pm \frac{(m + \phi/\pi)}{\sqrt{X_p^{(1)}}} \right]^2 \tag{4.6c}$$

Table 1. Extrapolated values of the sequences $\Lambda_n^{(0)}(\gamma, L, \phi)$ corresponding to the lowest eigenenergy in the sector n of the spin- $S = 1$ and $S = \frac{3}{2}$ chain. These estimates are obtained by using lattice sizes up to $L = 40$, and the conjectured results are given by (4.3) ($n = 0$) and (4.5) ($n \neq 0$).

	$n = 0, S = 1$			$n = 0, S = \frac{3}{2}$		
(γ, ϕ)	$(\pi/6, \pi/5)$	$(\pi/4, \pi/6)$	$(\pi/4, \pi/7)$	$(\pi/4, \pi/6)$	$(\pi/5, \pi/5)$	$(\pi/5, \pi/7)$
Extrapolated	0.015 00 (2)	0.013 888 (7)	0.010 204 (1)	0.416 66 (7)	0.037 500 (1)	0.019 132 (7)
Exact	0.015	0.0138	0.010 20408	0.0416	0.0375	0.019 132 65
	$n = 1, S = 1$			$n = 2, S = 1$		
(γ, ϕ)	$(\pi/5, \pi/8)$	$(\pi/5, \pi/6)$	$(\pi/6, \pi/5)$	$(\pi/6, \pi/8)$	$(\pi/6, \pi/6)$	$(\pi/5, \pi/5)$
Extrapolated	0.281 50 (8)	0.286 57 (1)	0.306 66 (5)	0.6725 (2)	0.6770 (8)	0.6166 (4)
Exact	0.281 5104	0.286 5741	0.306	0.672 525	0.677 083	0.616

The dimension and the spin of the composite field are given by

$$d_{\Delta_I, \bar{\Delta}_I}^{n, m+\phi/\pi} = \Delta_I + \bar{\Delta}_I + n^2 X_p^{(1)} + \frac{(m + \phi/\pi)^2}{16X_p^{(1)}} \tag{4.6d}$$

and

$$S_{\Delta_I, \bar{\Delta}_I}^{n, m+\phi/\pi} = \Delta_I - \bar{\Delta}_I + \frac{|n \cdot m|}{2} \tag{4.6e}$$

respectively. In fact we can interpret (4.5) as $d_{0,0}^{0,\phi/\pi}$ or $d_{1/16,1/16}^{0,\phi/\pi}$ depending on whether n is even or odd, respectively.

Let us now analyse some excited states. In table 2 we show for $(\gamma = \pi/5, \phi = \pi/5)$ and $(\gamma = \pi/5, \phi = \pi/4)$ some of our numerical estimates obtained from the extrapolations ($L \rightarrow \infty$) of the finite-size sequences corresponding to excited states. These results correspond to the dimensions $d_{1/2,1/2}^{(0,\phi/\pi)}$, $d_{0,1/2}^{1,\phi/\pi-1}$ and $d_{1/2,1/2}^{2,\phi/\pi}$ associated with the root distributions of figures 2(c), 2(e) and 2(g), respectively. The anomalous dimensions associated with figure 2(b) are $d_{0,0}^{0,\phi/\pi} + 2$ which correspond, in the periodic case, to the marginal operator responsible for the continuous changing of the exponents along the critical line. From these results, together with the results of the $\phi = 0$ chain [8] we conjecture, for the spin-1 chain in an L -even lattice with boundary angle ϕ , the following operator content

$$\zeta_{S=1}^e(\gamma, \phi) = \sum_{r=0}^1 \sum_{j=0}^1 Z_2(r, j) \sum_{\substack{n=2Z+r \\ m=2Z+j}} (\Delta_+^{(1)}, \Delta_-^{(1)})_{\text{KM}} \tag{4.7a}$$

where $(\Delta_+^{(1)}, \Delta_-^{(1)})_{\text{KM}}$ are the irreducible representations of a $U(1)$ Kac-Moody algebra with topological charge $k = 1$ and weights given by (4.6c). $Z_2(r, j)$ is the operator content of the sector $j = 0$ or 1 (parity even or odd) of the Ising model with toroidal boundary condition $r = 0$ or 1 (periodic or antiperiodic), which is given by

$$Z_2(0, 0) = (0, 0)_\vee + (1/2, 1/2)_\vee \tag{4.7b}$$

$$Z_2(0, 1) = Z_2(1, 0) = (1/16, 1/16)_\vee \tag{4.7c}$$

and

$$Z_2(1, 1) = (0, 1/2)_\vee + (1/2, 0)_\vee \tag{4.7d}$$

where $(\Delta_I, \bar{\Delta}_I)_\vee$ are the irreducible representations of the $c = \frac{1}{2}$ Virasoro algebra (Ising).

The result (4.7), together with the results of the periodic case [8] induce us to conjecture the following operator content for the general spin- S chain with boundary

Table 2. Extrapolated values for the mass gap amplitudes corresponding to some excited states of the spin-1 XXZ chain. These estimates are obtained by using lattice sizes up to $L = 40$, and the conjectured values are given by (4.6).

	$\gamma = \pi/5, \phi = \pi/5$			$\gamma = \pi/5, \phi = \pi/4$		
	$d_{1/2,1/2}^{0,\phi/\pi}$	$d_{0,1/2}^{1,\phi/\pi-1}$	$d_{1/2,1/2}^{2,\phi/\pi}$	$d_{1/2,1/2}^{0,\phi/\pi}$	$d_{0,1/2}^{1,\phi/\pi-1}$	$d_{1/2,1/2}^{2,\phi/\pi}$
Extrapolated	1.0166 (5)	0.9166 (4)	1.616 (4)	1.026 (1)	0.8843 (5)	1.626 (1)
Exact	1.016	0.916	1.616	1.026 041	0.884375	1.626 041

angle ϕ in a chain with L even

$$\zeta_S^e(\gamma, \phi) = \sum_{r=0}^{2S-1} \sum_{j=0}^{2S-1} Z_{2S}(r, j) \sum_{\substack{n=2SZ+r \\ m=2SZ+j}} (\Delta_+^{(S)}(\phi), \Delta_-^{(S)}(\phi)_{\text{KM}} \tag{4.8a}$$

where as before $(\Delta_+^{(S)}, \Delta_-^{(S)})_{\text{KM}}$ are the irreducible representations of $U(1)$ Kac-Moody algebra, with

$$\Delta_{\pm}^{(S)}(\phi) = \frac{1}{2} \left[n\sqrt{X_p^{(S)}} \pm \frac{(m + \phi S/\pi)}{4S\sqrt{X_p^{(S)}}} \right]^2 \quad X_p^{(S)} = \frac{\pi - 2S\gamma}{4\pi S} \tag{4.8b}$$

and $Z_{2S}(r, j)$ is the operator content of the sector $j = 0, 1, \dots, 2S - 1$ of the quantum $Z(2S)$ Fateev-Zamolodchikov Hamiltonian [9] with toroidal boundary condition $r = 0, 1, \dots, 2S - 1$. See, for example, [19] for an explanation of these boundary conditions. In the case where the lattice size L is an odd number our conjecture, for the operator content, is

$$\zeta_S^o(\gamma, \phi) = \sum_{r=0}^{2S-1} \sum_{j=0}^{2S-1} Z_{2S}(r, j) \sum_{\substack{n=2SZ+r+S \\ m=2SZ+j+S}} (\Delta_+^{(S)}, \Delta_-^{(S)})_{\text{KM}}. \tag{4.9}$$

To conclude this section it is interesting to observe, in comparison with the periodic case, that the toroidal boundary condition, specified by the angle ϕ , only changes the dimensions of the $U(1)$ Gaussian field by adding an extra vorticity of $\phi S/\pi$.

5. The scaling dimensions of extended algebras

As discussed in [10, 11], in the case of the spin- $S = \frac{1}{2}$ XXZ chain ($c = 1$), the effect of the boundary condition (2.3) corresponds, in the continuum model, to the introduction of external charges at infinity [1]. From this fact the whole operator content of the minimal models (1.1) and (1.2) ($c < 1$) can be obtained from the $S = \frac{1}{2}$ XXZ chain by choosing properly the constant of anisotropy γ and the boundary angle ϕ [11].

As we already know, from the results of the periodic case, the conformal anomaly for the spin- S XXZ chain is $c = 3S/1 + S$, for $0 \leq \gamma \leq \pi/2S$, and we will see now that, in the same way as in the $S = \frac{1}{2}$ case, we can also relate this model, with the boundary condition (2.3), to models having $c < 3S/(1 + S)$. Suppose now that, for a given lattice size L , part of the eigenspectrum (including the ground-state energy) of the spin- S XXZ chain, with boundary conditions specified the angle ϕ , is equal up to order $o(L^{-1})$, to the eigenspectrum of a different model with periodic boundary condition. This is exactly the case of the spin- $S = \frac{1}{2}$. In this case the operator content derived in the last section, together with the relations (1.8) and (1.9), would give us the conformal anomaly and scaling dimensions of the operators of this different model.

From the results (4.3) and (4.4) of the last section and the fact that the conformal anomaly of the spin- S XXZ chain is $c = 3S/(1 + S)$ we obtain, from (1.8), that the ground-state energy $E_0^{(0)}(\gamma, L, \phi)$ of the spin- S XXZ chain, with boundary angle ϕ , behaves as ($0 \leq \gamma \leq \pi/2S$)

$$\frac{E_0^{(0)}(\gamma, L, \phi)}{L} = e_\infty(\gamma, L) - \frac{\zeta\pi}{6L^2} \left\{ \frac{3S}{1+S} - \frac{3S\phi^2}{\pi(\pi - 2S\gamma)} \right\} + o(L^{-2}) \tag{5.1}$$

where, as before, $e_\infty(\gamma, L)$ is the ground-state energy per particle in the infinite-size limit and ζ is the sound velocity given by (4.2). From (1.8) and the above considerations $E_0^{(0)}(\gamma, \lambda, \phi)$ is related to a periodic critical quantum chain with conformal anomaly

$$c(\gamma, \phi) = \frac{3S}{1+S} \left\{ 1 - \frac{(1+S)\phi^2}{\pi(\pi-2S\gamma)} \right\}. \tag{5.2}$$

If we now choose

$$\gamma = \frac{\pi}{m+k} \quad \phi = 2\gamma, m = 3, 4, \dots \tag{5.3}$$

with $k = 2S$, we obtain

$$c = \frac{3k}{2+k} \left\{ 1 - \frac{2(2+k)}{m(m+k)} \right\} \quad m = 3, 4, \dots \tag{5.4}$$

which is the conformal anomaly of the general conformal series (1.6).

The conformal dimensions (1.7) can also be obtained from the operator content of the spin- S XXZ chain. For example, we will show that the mass gap amplitudes of the sector with $n = 0$ will give us the scalar operators $(\Delta_{p,q} = \bar{\Delta}_{p,q})$ of the extended theories (1.6). From (4.8) the operator content for this section, with boundary condition ϕ , is given by

$$G^{(n=0)}(\gamma, \phi) = \sum_{r=0}^{2S-1} \sum_{m=2SZ+r} Z_{2S}(r, 0) (\Delta_m^{(S)}(\phi), \Delta_m^{(S)}(\phi))_{KM} \tag{5.5a}$$

where

$$\Delta_m^{(S)}(\phi) = \frac{(m + \phi S / \pi)^2}{8S(1 - 2S\gamma / \pi)} \tag{5.5b}$$

and $Z_{2S}(r, 0)$ is the operator content of the sector $j = 0$ (parity zero) of the $Z(2S)$ Fateev-Zamolodchikov Hamiltonian [19] with boundary conditions $r = 0, 1, \dots, 2S - 1$.

From previous analysis we know [19] that the lowest dimensions appearing in $Z_{2S}(r, 0)$ correspond to $(\Delta_{2S}^{(r)}, \Delta_{2S}^{(r)})$ where

$$\Delta_{2S}^{(r)} = \frac{r(2S-r)}{8S(S+1)} \quad r = 0, 1, \dots, 2S-1 \tag{5.6}$$

which are the dimensions of the r th-order parameter of the $Z(2S)$ Fateev-Zamolodchikov model [4]. As a consequence (5.5) contains the particular set of dimensions

$$h_m(\gamma, \phi) = 2(\Delta_{2S}^{(r)} + \Delta_m^{(S)}(\phi)) \tag{5.7}$$

where $m = 0, 1, 2, \dots; r = m \pmod{2S}$, $\Delta_{2S}^{(r)}$ and $\Delta_m^{(S)}$ are given by (5.5b) and (5.6). Let us now define the following difference of dimensions

$$\tilde{\Delta}_{p-q}^q(\gamma, \phi) = h_{p-q}(\gamma, q\phi) - h_0(\gamma, \phi) = \frac{[(p-q) + \phi Sq / \pi]^2 - (\phi S / \pi)}{4S(1 - 2S\gamma / \pi)} + \frac{t(2S-t)}{4S(S-1)} \tag{5.8}$$

where $p > q$ and $t = (p - q) \pmod{2S}$. If we now make the choice (5.3) for γ and ϕ we obtain, with $k = 2S$:

$$\tilde{\Delta}_{p-q}^q = \frac{[p(m+k) - qm]^2 - k^2}{2km(m+k)} + \frac{t(k-t)}{k(k+2)} \tag{5.9}$$

which is precisely the dimensions of the scalar operators predicted in (1.7) for the general theories (1.6).

Before we close this paper it is interesting to remark here that in the $S = \frac{1}{2}$ XXZ chain it was possible to obtain [11] not only the scaling dimensions of the operators of the minimal models, like in (5.8) and (5.9), but also the characters of the minimal conformal algebras. Surprisingly in the spin- $S = \frac{1}{2}$ quantum chain the numerical results for finite chains [11] show us that due to an exact cancellation of the levels of different sectors and boundaries the partition function of the minimal models, in finite lattice chains, are obtained from these of the spin- $\frac{1}{2}$ XXZ chain. This exact cancellation of levels is related to the fact that the exact integrability of the model does not depend on the lattice size [20]. The same type of cancellation also occurs for the general spin- S chain. For example we can show that all the solutions $\{\lambda\}$ of the BAE (2.4) in the sector $(n+1)$ with boundary conditions $\phi = 2\gamma k$ ($k = 0, 1, 2, \dots$) is also a solution of the same equations in the sector n and boundary condition $\phi = 2\gamma(k+1)$, if we add one λ at infinity. The corresponding eigenenergies are the same because the zero at infinity does not contribute to the energy, as we can see from (2.5). We expect therefore that the same types of relations between finite systems obtained in the $S = \frac{1}{2}$ case can also be derived for the general spin- S chain. A possible way to proceed in this investigation is the use of quantum algebras, as in [20].

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References

- [1] Belavin A A, Polyakov A M and Zamolodchikov A B 1984 *J. Stat. Phys.* **34** 763; *Nucl. Phys. B* **241** 333
- [2] Friedan D, Qiu Z and Shenker S 1984 *Phys. Rev. Lett.* **52** 1575
- [3] Bershadsky M A, Knizhnik V G and Teitelman M G 1984 *Phys. Lett.* **151B** 31
Friedan D, Qiu Z and Shenker S 1985 *Phys. Lett.* **151B** 37
- [4] Zamolodchikov A B and Fateev V A 1985 *Zh. Eksp. Teor. Fiz.* **89** 380; *Sov. Phys.-JETP* **62** 215
- [5] Knizhnik V G and Zamolodchikov A B 1984 *Nucl. Phys. B* **247** 83
- [6] Kastor D, Martinec E and Qiu Z 1988 *Phys. Lett. B* **200** 434
Bagger J, Nemechansky D and Yankielowicz S 1988 *Phys. Rev. Lett.* **60** 389
Ravanini F 1988 *Mod. Phys. Lett. A* **3** 271
- [7] Feigin B L and Fuchs K B 1982 *Funct. Anal. Appl.* **16** 114
Dotsenko VI S and Fateev V A 1984 *Nucl. Phys. B* **240** 312
- [8] Alcaraz F C and Martins M J 1988 *Phys. Rev. Lett.* **61** 1529; 1989 *J. Phys. A: Math. Gen.* **22** 1829
- [9] di Francesco P, Saleur H and Zuber J-B 1988 *Nucl. Phys. B* **300** [FS22]
- [10] Alcaraz F C, Barber M N and Batchelor M T 1987 *Phys. Rev. Lett.* **8** 771; 1988 *Ann. Phys., NY* **182** 280
- [11] Alcaraz F C, Grimm U and Rittenberg V 1989 *Nucl. Phys. B* **316** 735
Alcaraz F C, Baake M, Grimm U and Rittenberg V 1989 *J. Phys. A: Math. Gen.* **22** L5
- [12] Cardy J L 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55
- [13] Blöte H W, Cardy J L and Nightingale M P 1986 *Phys. Rev. Lett.* **56** 742
Affeck I 1986 *Phys. Rev. Lett.* **56** 746
- [14] Yang C N and Yang C P 1966 *Phys. Rev.* **150** 321, 327
- [15] Zamolodchikov A B and Fateev V A 1980 *Sov. J. Nucl. Phys.* **32** 2
- [16] Sogo K 1984 *Phys. Lett. A* **104** 51
Babudjian H M and Tselik A M 1985 *Nucl. Phys. B* **265** [FS15] 24
Kirillov A N and Reshetikhin 1987 *J. Phys. A: Math. Gen.* **20** 1565, 1585

- [17] Takhtajan L 1982 *Phys. Lett.* **87A** 479
Babujian J 1982 *Phys. Lett.* **90A** 479; 1983 *Nucl. Phys. B* **215** [FS7] 317
- [18] de Vega H J and Karowski M 1987 *Nucl. Phys. B* **285** 619
Karowski M 1988 *Nucl. Phys. B* **300** [FS22] 473
- [19] Alcaraz F C and Lima Santos A 1986 *Nucl. Phys. B* **274** [FS17] 436
Alcaraz F C 1987 *J. Phys. A: Math. Gen.* **20** 2511, L623
- [20] Pasquier V and Saleur H 1989 *Preprint SphT/89 031*