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LETTER TO THE EDITOR

Operator content of the *XXZ* chain

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Abstract. The finite-size scaling spectra of the *XXZ* Heisenberg chain are presented for even and odd numbers of sites, respectively. The operator content is given for free as well as for toroidal boundary conditions.

The *XXZ* model is defined by the Hamiltonian

$$H=-\frac{\gamma}{2\pi\sin\gamma}\sum_{j=1}^{N}(\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y-\cos\gamma\sigma_j^z\sigma_{j+1}^z)\qquad(0\leqslant\gamma<\pi)\tag{1}$$

where σ^x, σ^y and σ^z are Pauli matrices. The properties of its finite-size scaling spectrum have recently been investigated by several authors using both analytic and numerical methods (Alcaraz *et al* 1987a, b, c, Hamer *et al* 1987, Hamer and Batchelor 1988, Woynarovich 1987). It is the aim of this letter to give a conjecture for the whole operator content of the model for various boundary conditions (BC). This conjecture is based on all previously known results, on further numerical studies (Bethe ansatz calculations with numerical solution of the transcendental equations as well as ordinary finite-size calculations up to 18 sites) and on extended modular invariance.

The global symmetry of the infinite system is O(2). In the basis

$$\sigma_j^{\pm 1}=\sigma_j^x\pm \mathrm{i}\sigma_j^y\qquad \sigma_j^0=\sigma_j^z\tag{2}$$

the Hamiltonian is invariant under the transformations

$$\sigma_j'^m=\sum_{n=-1}^{1}A^{mn}\sigma_j^n\tag{3}$$

where the matrices A^{mn} form the O(2) group

$$\mathscr{G}=\{G(\vartheta)C^\alpha\,|\,\vartheta\in[0,2\pi),\,\alpha=0,1\}\simeq \mathrm{O}(2)\tag{4}$$

where

$$G(\vartheta)=\begin{pmatrix}\mathrm{e}^{-\mathrm{i}\vartheta}&0&0\\0&1&0\\0&0&\mathrm{e}^{\mathrm{i}\vartheta}\end{pmatrix}\qquad C=\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix}.\tag{5}$$

We now specify the boundary conditions for the Hamiltonian (1).

(a) Free boundary conditions (H^{F})

$$\sigma_{N+1}^x=\sigma_{N+1}^y=\sigma_{N+1}^z=0.\tag{6}$$

(b) Toroidal boundary conditions (H^B)

$$\sigma^m_{N+1} = \sum_{n=-1}^{1} B^{mn}\sigma^n_1 \tag{7}$$

where B is one of the matrices of (4). Two Hamiltonians H^{B_1} and H^{B_2} have the same spectrum if the group elements B_1 and B_2 belong to the same conjugacy class. The conjugacy classes of O(2) are as follows.

$$\begin{aligned} &(\mathrm{I}): \{\mathbb{1}\} \qquad (\mathrm{II}): \{G(\pi)\} \qquad (\mathrm{III}): \{G(\vartheta), G(-\vartheta)\} \qquad \forall\vartheta \neq 0, \pi \\ &(\mathrm{IV}): \{G(\vartheta)C \,|\, \vartheta \in [0, 2\pi)\}. \end{aligned} \tag{8}$$

The global symmetry of the Hamiltonian with free BC (H^F) is O(2). The same is true for periodic ($B = \mathbb{1}$) and antiperiodic ($B = G(\pi)$) BC. The symmetry for the elements of the conjugacy classes (III) is $SO(2) = \{G(\vartheta) | \vartheta \in [0, 2\pi)\}$ and for the Hamiltonian H^B where B is one of the elements of the conjugacy class (IV), e.g., $G(\vartheta)C$, it is only $Z_2 \otimes Z_2 = \{\mathbb{1}, G(\vartheta)C, G(\pi), G(\pi+\vartheta)C\}$. (These are the symmetries for an *even* number of sites; for an *odd* number of sites one has to keep in mind that one has spin-$\frac{1}{2}$ waves.)

Before we present our results, let us specify the notation (see von Gehlen *et al* (1988) for further details). Since the central charge of the Virasoro algebra is $c = 1$ for the Hamiltonian (1), the operator content for free BC will be given in terms of primary operators (Δ) of the U(1) Kac–Moody algebra with a character function

$$\chi_\Delta(z) = \mathrm{Tr}(z^{L_0}) = z^\Delta \prod_{m=1}^{\infty} \frac{1}{1 - z^m}. \tag{9}$$

The operator content for the Hamiltonian with BC (7) will be given in terms of primary operators ((Δ), ($\bar{\Delta}$)) of two commuting U(1) Kac–Moody algebras.

The finite-size scaling limits of the spectra have to be computed separately for even numbers of sites (N) and odd numbers of sites. The operator content for an odd number of sites will be given taking as a reference energy the ground-state energy for an even number of sites. For example, if one takes free boundary conditions and the ground-state energies for N sites are $E^F_0(N)$, we take as reference energy for $2N+1$ sites

$$E^F_R(2N+1) = \tfrac{1}{2}(E^F_0(2N) + E^F_0(2N+2)) \tag{10}$$

and consider $E^F_c(2N+1) - E^F_R(2N+1)$ as the first energy gap. For toroidal BC all energies are related to the ground-state energy of the system with *periodic* BC and an even number of sites.

The charge operator which commutes with the Hamiltonian (except in the case when the BC belongs to the conjugacy class (IV)) is

$$\hat{Q} = \tfrac{1}{2} \sum_{j=1}^{N} \sigma^z_j. \tag{11}$$

Notice that the eigenvalues (Q) are integer (half-integer) when N is even (odd).

It turns out that the dependence of the operator content on the coupling constant (see (1)) is simpler when it is expressed in terms of

$$h = \frac{\pi}{4(\pi - \gamma)} \qquad (\infty > h \geq \tfrac{1}{4}). \tag{12}$$

We now list the operator content for various BC.

(i) *Free boundary conditions.* If we denote by $\mathscr{E}_Q^{\mathrm{F}}$ the operator content for the charge sector Q we have

$$\mathscr{E}_Q^{\mathrm{F}} = (Q^2/4h) \tag{13}$$

where Q is an integer or half-integer.

(ii) *Toroidal boundary conditions.* The operator content for the conjugacy classes (I), (II) and (III) can be given in a compact form. With the notation

$$\sigma_{N+1}^{\pm 1} = \mathrm{e}^{\pm 2\pi i l}\sigma_1^{\pm 1} \qquad 0 \leqslant l < 1 \qquad \sigma_{N+1}^{0} = \sigma_1^{0} \tag{14}$$

the operator content in the charge Q sector is

$$\mathscr{E}_Q^{l} = \bigoplus_{m \in \mathbb{Z}} \left(\left(\frac{[Q+4h(l+m)]^2}{16h} \right), \left(\frac{[Q-4h(l+m)]^2}{16h} \right) \right) \tag{15}$$

where Q is an integer or half-integer.

For the conjugacy class (IV) (we take the BC given by the charge conjugation C transformation (4) as a typical element), we have for N *even*

$$\begin{aligned} \mathscr{E}^C_{C=+,G(\pi)=+} = \mathscr{E}^C_{C=+,G(\pi)=-} &= (\{\tfrac{1}{16}\}, \{\tfrac{1}{16}\}) \oplus (\{\tfrac{9}{16}\}, \{\tfrac{9}{16}\}) \\ \mathscr{E}^C_{C=-,G(\pi)=+} = \mathscr{E}^C_{C=-,G(\pi)=-} &= (\{\tfrac{1}{16}\}, \{\tfrac{9}{16}\}) \oplus (\{\tfrac{9}{16}\}, \{\tfrac{1}{16}\}). \end{aligned} \tag{16}$$

Here, $G(\pi) = \pm$, $C = \pm$ are the eigenvalues of the $G(\pi)$ and C operators which generate the $Z_2 \otimes Z_2$ symmetry of the boundary condition C and

$$\{\tfrac{1}{16}\} = \bigoplus_{m \in \mathbb{Z}} \left(\frac{(1+8m)^2}{16} \right) \qquad \{\tfrac{9}{16}\} = \bigoplus_{m \in \mathbb{Z}} \left(\frac{(3+8m)^2}{16} \right). \tag{17}$$

For N *odd* we have

$$\mathscr{E}^C_{C=+} = \mathscr{E}^C_{C=-} = (\{\tfrac{1}{16}\} \oplus \{\tfrac{9}{16}\}, \{\tfrac{1}{16}\} \oplus \{\tfrac{9}{16}\}). \tag{18}$$

Here, the eigenvalues of C and $G(\pi)$ cannot be measured simultaneously which is a consequence of the spin-$\frac{1}{2}$ waves.

Now let us give some justification for expressions (13), (15), (16) and (18). First of all the finite-size spectrum for N even (Q is an integer in (13) and (15) as well as (16)) can be obtained as the large-n limit of the Z_n models (see von Gehlen *et al* 1988). The dimensions of (15) (again where Q is an integer) also satisfy the conditions of extended modular invariance (Suranyi 1987). We could not find similar arguments for half-integer Q but we have checked (Baake *et al* 1987) that for the points $h = N^2/4$ where one has SU(2) Kac–Moody symmetry, the sectors with half-integer charge give representations of shifted SU(2) Kac–Moody algebras.

The analytic expressions for the operator content of the XXZ chain allow one to clarify the known connection between this model and other models with $c < 1$. This is going to be the subject of another publication.

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