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LETTER TO THE EDITOR

The modified *XXZ* Heisenberg chain, conformal invariance and the surface exponents of $c<1$ systems

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Abstract. We present the operator content of the *XXZ* chain in the presence of external fields. The finite-size scaling spectra can be expressed in terms of irreps of shifted U(1) Kac–Moody algebras, the shift depending on the external fields. Using an explicit Feigin–Fuchs construction, we project out from these spectra the operator content of $c<1$ systems with free, fixed and mixed boundary conditions. We also show how this projection mechanism works for a finite number of sites.

The modified *XXZ* model with N sites is defined by the Hamiltonian

$$H=-\frac{\gamma}{2\pi\sin(\gamma)}\left\{\sum_{j=1}^{N-1}\left[\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y-\cos(\gamma)\,\sigma_j^z\sigma_{j+1}^z\right]\right.$$
$$\left.+\sin(\gamma)\left[\tan\left(\frac{\omega+\delta}{2}\right)\sigma_1^z+\tan\left(\frac{\omega-\delta}{2}\right)\sigma_N^z\right]\right\} \qquad (1)$$

where σ^x, σ^y and σ^z are Pauli matrices, and ω and δ describe the coupling of the external fields. (For the special case $\omega=\delta=0$ we get the *XXZ* chain with free boundary conditions (BC) for which the operator content is already known (Alcaraz *et al* 1988a and references therein).)

Instead of describing the anisotropy in the Hamiltonian H through the parameter γ it is useful to define

$$h=\tfrac{1}{4}(1-\gamma/\pi)^{-1} \qquad h\geq\tfrac{1}{4}. \qquad (2)$$

As discussed by Baake *et al* (1988), h is related to the compactification radius R of the bosonic string ($h=\tfrac{1}{2}R^2$). We notice that the charge operator

$$\hat{Q}=\tfrac{1}{2}\sum_{j=1}^{N}\sigma_j^z$$

commutes with H and that its eigenvalues Q are integer (half integer) when N is even (odd). Let $E_{Q;i}(N)$ be the energy levels, $i=0,1,\ldots$, in the charge Q sector of the

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Hamiltonian with N sites and $E_0^{\mathrm{F}}(N)$ the ground-state energy of the Hamiltonian with free BC. We consider the following quantities:

$$\begin{aligned}\bar{E}_{Q;i}&=(N/\pi)(E_{Q;i}(N)-E_0^{\mathrm{F}}(N))\\ \mathscr{E}_Q(N,z)&=\sum_i z^{\bar{E}_{Q;i}(N)}\\ \mathscr{E}_Q(z)&=\lim_{N\to\infty}\mathscr{E}_Q(N,z).\end{aligned}\tag{3}$$

Using numerical estimates from chains up to 18 sites as well as analytical methods (Batchelor 1988, Hamer and Batchelor 1988) we obtained the following ansatz:

$$\mathscr{E}_Q(z)=z^{(Q+\varphi)^2/4h}\Pi_V(z)\tag{4}$$

$$\Pi_V(z)=\prod_{m=1}^{\infty}(1-z^m)^{-1}\tag{5}$$

where $\varphi=-2h\omega/\pi$ is independent of δ (see equation (1)) and Q is integer or half integer for N even or odd, respectively. This result is very interesting because it implies that the operator content in the charge Q sector is given by a single irrep of a shifted U(1) Kac–Moody algebra (Baake *et al* 1988) the shift φ being related to ω. The expression (4) is the starting point of the Feigin–Fuchs construction (Feigin and Fuchs 1982, Dotsenko and Fateev 1984) of irreps of Virasoro algebras with $c<1$ starting from irreps for $c=1$ (this is the central charge of the XXZ chain). This construction will allow us to identify the operator content of systems with $c<1$ with free, fixed and mixed BC. First, we recall that for $c<1$ the central charge is quantised:

$$c=1-6/m(m+1)\qquad m=3,4,\ldots\tag{6}$$

and for a given m, the highest weights $\Delta_{r,s}$ (i.e. the lowest eigenvalues of the Virasoro generator L_0) of unitary irreps are also quantised:

$$\Delta_{r,s}=\frac{[(m+1)r-ms]^2-1}{4m(m+1)}\qquad 1\leqslant r\leqslant m-1;\ 1\leqslant s\leqslant m.\tag{7}$$

The corresponding character functions are (Rocha-Caridi 1985)

$$\begin{aligned}\chi_{r,s}&=\mathrm{Tr}(z^{L_0})=\Omega_{r,s}-\Omega_{r,-s}\\ \Omega_{r,s}&=\sum_{\alpha\in Z}z^{\{[2m(m+1)\alpha+(m+1)r-ms]^2-1\}/4m(m+1)}\Pi_V(z).\end{aligned}\tag{8}$$

In order to apply the Feigin–Fuchs procedure, let us assume that we have fixed h and φ. Instead of considering $E_0^{\mathrm{F}}(N)$ as ground-state energy (see equation (3)), we take as ground-state energy $E_{0;0}(N)$, i.e. the ground state in the charge-zero sector of the Hamiltonian (1) (with h, ω and δ fixed). Next, instead of considering charges taking values in $\boldsymbol{Z}$ or $\boldsymbol{Z}+\frac{1}{2}$, it is convenient to work with charges in $\boldsymbol{Z}_n$ or $\boldsymbol{Z}_n+\frac{1}{2}$, respectively (the value of n will be fixed later). Thus, instead of (3) and (4) we have

$$\begin{aligned}\bar{F}_{q;i}&=(N/\pi)(E_{q;i}(N)-E_{0;0}(N))\\ \mathscr{F}_q(N,z)&=\sum_i z^{\bar{F}_{q;i}}\\ \mathscr{F}_q(z)&=\lim_{N\to\infty}\mathscr{F}_q(N,z)=\sum_{\alpha\in Z}z^{[(n\alpha+q+\varphi)^2-\varphi^2]/4h}\Pi_V(z)\end{aligned}\tag{9}$$

where $q=0,1,\ldots,n-1$ for N even and $q=\frac{1}{2},\frac{3}{2},\ldots,n-\frac{1}{2}$ for N odd. We now choose

$$h=\frac{n^2}{4m(m+1)} \qquad \varphi=\frac{n}{2m(m+1)} \tag{10}$$

and get

$$\begin{aligned}\mathscr{F}_q(z)&=\sum_{\alpha\in Z} z^{[(2m(m+1)\alpha+2m(m+1)q/n+1)^2-1]/4m(m+1)}\Pi_V(z)\\&=\mathscr{F}_{q\pm n}(z).\end{aligned} \tag{11}$$

This expression resembles $\Omega_{r,s}$ of (8) if n is a divisor of $2m(m+1)$. Since the finite-size scaling spectrum given by (4) remains positive for any positive h, we will assume that we can use the equations above also for $0<h\leqslant\frac{1}{4}$ (see equation (2)). The four choices of n given in table 1 divide the domain $h\geqslant\frac{1}{6}$ into four regions which correspond to the p-state Potts models, tricritical Potts model, O(p) models and low temperature O(p) models (Nienhuis *et al* 1983, Nienhuis 1984, Saleur 1987, di Francesco *et al* 1987, Batchelor and Blöte 1988 and references therein). A more detailed discussion of these models based on the Feigin–Fuchs construction when applied to toroidal BC will be given elsewhere (Alcaraz *et al* 1988c). Let us first consider the case of the p-state Potts model ($n=m+1$). Comparing (8) and (11) we have

$$\mathscr{F}_{-q}=\Omega_{1,2q+1} \tag{12}$$

and

$$\chi_{1,2v+1}=\mathscr{F}_{-v}-\mathscr{F}_{v+1} \qquad q \text{ integer} \tag{13}$$

$$\chi_{1,2v}=\mathscr{F}_{1/2-v}-\mathscr{F}_{1/2+v} \qquad q \text{ half-integer.} \tag{14}$$

In order to clarify the physical significance of our result, let us take $m=3$, $n=4$ (q integer). We find

$$\begin{aligned}\chi_{1,1}&=\mathscr{F}_0-\mathscr{F}_1 \qquad &\Delta=0\\ \chi_{1,3}&=\mathscr{F}_{-1}-\mathscr{F}_2 \qquad &\Delta=\tfrac{1}{2}.\end{aligned} \tag{15}$$

These are precisely the surface exponents of the Ising model (or, alternatively, the exponents for fixed BC which are identical) (Cardy 1986, von Gehlen and Rittenberg 1986). If we take q half integer we have

$$\chi_{1,2}=\mathscr{F}_{-1/2}-\mathscr{F}_{3/2} \qquad \Delta=\tfrac{1}{16} \tag{16}$$

which corresponds to the case of mixed BC (Cardy 1986). We now consider $m=5$, $n=6$ (the three-state Potts model) and q integer. We obtain

$$\begin{aligned}\chi_{1,1}&=\mathscr{F}_0-\mathscr{F}_1 \qquad &\Delta=0\\ \chi_{1,3}&=\mathscr{F}_{-1}-\mathscr{F}_2 \qquad &\Delta=\tfrac{2}{3}\\ \chi_{1,5}&=\mathscr{F}_{-2}-\mathscr{F}_3 \qquad &\Delta=3.\end{aligned} \tag{17}$$

These are again the known surface exponents (free BC) or the exponents corresponding to fixed BC. If we take q half integer we find

$$\begin{aligned}\chi_{1,2}&=\mathscr{F}_{-1/2}-\mathscr{F}_{3/2} \qquad &\Delta=\tfrac{1}{8}\\ \chi_{1,4}&=\mathscr{F}_{-3/2}-\mathscr{F}_{5/2} \qquad &\Delta=\tfrac{13}{8}.\end{aligned} \tag{18}$$

Table 1. Definition of the models. The arguments of the cosine functions are taken positive. The values of n occur in (10).

	p-state Potts $0<p\leqslant 4$	Tricritical p-state Potts $0<p\leqslant 4$	O(p) $-2<p\leqslant 2$	Low temperature O(p) $-2<p\leqslant 2$
Definition of the model	$\frac{1}{2}\sqrt{p}=\cos\pi(1-1/4h)$	$\frac{1}{2}\sqrt{p}=\cos\pi(1/4h-1)$	$\frac{1}{2}p=\cos\pi(1/h-1)$	$\frac{1}{2}p=\cos\pi(1-1/h)$
Domain of h	$\frac{1}{2}\geqslant h\geqslant\frac{1}{4}$	$\frac{1}{4}\geqslant h\geqslant\frac{1}{6}$	$1\geqslant h\geqslant\frac{1}{2}$	$h\geqslant 1$
Values of n	$m+1$	m	$2m$	$2(m+1)$

Table 2. The operator contents for free (fixed) and mixed boundary conditions and their relation to the XXZ chain for various models. (For the p-state Potts case see (12)–(14)).

	p-state Potts	Tricritical p-state Potts	O(p) (m odd)	Low-temperature O(p) (m even)
	$\mathcal{F}_{-q}=\Omega_{1,2q+1}$	$\mathcal{F}_{q}=\Omega_{2q+1,1}$	$\mathcal{F}_{q}=\Omega_{q+1,1}$	$\mathcal{F}_{-q}=\Omega_{q+1}$
Free (fixed) BC	$\chi_{1,2v+1}=\mathcal{F}_{-v}-\mathcal{F}_{v+1}$	$\chi_{1+2v,1}=\mathcal{F}_{v}-\mathcal{F}_{-v-1}$	$\chi_{r,1}=\mathcal{F}_{r-1}-\mathcal{F}_{-r-1}$	$\chi_{1,s}=\mathcal{F}_{1-s}-\mathcal{F}_{1+s}$
Mixed BC	$\chi_{1,2v}=\mathcal{F}_{-v+1/2}-\mathcal{F}_{v+1/2}$	$\chi_{2v,1}=\mathcal{F}_{v-1/2}-\mathcal{F}_{-v-1/2}$	$\chi_{r,\frac{1}{2}(m-1)}=\mathcal{F}_{\frac{1}{2}m-1-r}-\mathcal{F}_{\frac{1}{2}m-1+r}$	$\chi_{\frac{1}{2}m-1,s}=\mathcal{F}_{\frac{1}{2}(1-m)+s}-\mathcal{F}_{\frac{1}{2}(1-m)-s}$

The values $\Delta = \frac{1}{8}$ and $\frac{13}{8}$ are indeed the exponents of the three-state Potts model with mixed BC (Cardy 1986). The case $m = 4$ does not correspond to the tricritical Ising model. It has the same operator content for periodic BC as the tricritical Ising model but with another distribution of the operators between the charge sectors (Alcaraz *et al* 1988c) so we have nothing with which to compare the $m = 4$ case.

From the above considerations we will assume that for all m, (13) gives us the surface (or fixed boundary condition) exponents and (14) the exponents for mixed BC. There are two supplementary arguments in favour of this assumption. First, we notice that, in agreement with an earlier result of Cardy (1984), we get $\Delta_{1,3}$ for the leading surface exponent from (13). Second, if we start with the Potts models with free or fixed BC, use the Temperley–Lieb algebra (Temperley and Lieb 1971, Pasquier 1987) and then take the representation of the algebra in terms of Pauli matrices, we get the Heisenberg chain with an even number of sites but an *imaginary* external field (Alcaraz 1988b). If we repeat the same procedure starting with mixed BC we get the Heisenberg chain with an odd number of sites.

The operator contents for free (fixed) and mixed BC for various models are given in table 2. Let us derive some known results. For the tricritical Ising model ($m = n = 4$) we get

$$\text{free BC} \qquad (0) + (\tfrac{3}{2}) \tag{19}$$

$$\text{mixed BC} \qquad (\tfrac{7}{16}). \tag{20}$$

Equation (19) is in agreement with the result of Cardy (1986); equation (20) is new. In the case of the $O(p)$ models, the leading surface exponent is $\Delta_{2,1}$, again in agreement with Cardy (1984).

Let us proceed with the discussion of our results by means of an example. From the first line of (17) we can see that combining the finite-size scaling spectra of the $q = 0$ and $q = 1$ sectors (see equation (9)), disregarding all the doublets (levels which occur in the sector $q = 0$ and $q = 1$) and keeping only the singlets (levels which occur only in the $q = 0$ sector), we obtain the vacuum sector of the three-state Potts model with free BC. This is the general structure of the projection mechanism of the finite-size scaling spectra for $c < 1$ from the spectra for $c = 1$. We can go one step further and check whether the same projection mechanism also works for a finite number of sites. For the example of (17), this would imply that all the levels of the sector $q = 1$ are exactly degenerate with levels of $q = 0$ even for a finite number of sites, and the remaining levels in $q = 0$ (which have no correspondent in $q = 1$) define the spectrum of the vacuum sector of the three-state Potts model. The same picture should be valid for the $q = -1$ and $q = 2$ sectors as well as for the $q = -2$ and $q = 3$ sectors. In table 3 we give the values of $\bar{F}_{q,i}$ (see equation 9) for four sites ($h = \frac{3}{10}$, $\omega = -\frac{1}{6}\pi$) and two values of δ. Let us compare the sectors with $q = 0$ and $q = 1$. For $\delta = 0$ we have in the $q = 0$ sector levels which are degenerate with levels in the $q = 1$ sector. Most of these values change with δ but some do not. (Note that the latter phenomenon does not yet occur in the simple example of table 3.) All these doublets have to be projected out. Then there are levels in the $q = 0$ sector which do not appear in the $q = 1$ sector and whose values are independent of δ. These singlets have to be kept. The same picture is valid for the $q = -1$ ($q = 2$) and $q = -2$ ($q = 3$) sectors. The remaining spectrum (given by the singlets) is exactly the spectrum of the three-state Potts model with free (fixed) BC (see table 2 of von Gehlen *et al* 1987) and two sites. We have checked that the same mechanism works for any number of sites and for all the models

Table 3. Table of $\bar{F}_{q,i}(N)$ values (equation ((9)) for $N=4$, $h=\frac{3}{10}$, $\omega=-\frac{1}{6}\pi$ and two values of δ. The spectra for $q=0$, ±1, ±2 and 3 are given. The underlined levels occur in the three-state Potts model with 2 sites and free BC. (The XXZ chain with $2N$ sites gives the p-state Potts models with N sites and free BC.)

$\delta=0$		$\delta=\omega$	
$q=0$	$q=1$	$q=0$	$q=1$
0.000 000		0.000 000	
0.566 777	0.566 777	0.573 943	0.573 943
1.124 431	1.124 431	1.128 282	1.128 282
1.407 619		1.407 619	
1.689 669	1.689 669	1.693 423	1.693 423
1.980 841	1.980 841	1.992 459	1.992 459
$q=-1$	$q=2$	$q=-1$	$q=2$
0.471 151		0.471 151	
1.071 362		1.071 362	
1.671 573		1.671 573	
1.920 189	1.920 189	1.928 985	1.928 985
$q=-2$	$q=3$	$q=-2$	$q=3$
1.806 467		1.806 467	

(any m with $n=m+1$) belonging to the p-state Potts class. As a further example of the projection mechanism, in table 4 we illustrate the case of the Ising model ($m=3$, $n=4$). Here we use (15).

In the case of an odd number of sites, the energy gaps ($E_{q;i}(2N+1)-E_{-1/2;0}(2N+1)$) of the XXZ chain are related to the energy gaps of the Potts model

Table 4. Table of $\bar{F}_{q,i}(N)$ values (equation (9)) for $N=4$, $h=\frac{1}{3}$, $\omega=-\frac{1}{4}\pi$ and three values of δ. The spectra for $q=0$, ±1, and 2 are given. The underlined levels occur in the Ising model with two sites and free BC (von Gehlen and Rittenberg 1986). Note that one of the degenerate levels in the $q=-1$ and $q=2$ sectors is independent of δ.

$\delta=0$		$\delta=\frac{1}{2}\omega$		$\delta=\omega$	
$q=0$	$q=1$	$q=0$	$q=1$	$q=0$	$q=1$
0.000 000		0.000 000		0.000 000	
0.610 592	0.610 592	0.619 855	0.619 855	0.650 912	0.650 912
1.143 009	1.143 009	1.147 882	1.147 882	1.164 809	1.164 809
1.423 525		1.423 525		1.423 525	
1.713 250	1.713 250	1.721 434	1.721 434	1.750 846	1.750 846
2.081 149	2.081 149	2.095 750	2.095 750	2.145 273	2.145 273
$q=-1$	$q=2$	$q=-1$	$q=2$	$q=-1$	$q=2$
0.393 453		0.393 453		0.393 453	
1.030 072		1.030 072		1.030 072	
1.666 692	1.666 692	1.666 692	1.666 692	1.666 692	1.666 692
1.930 389	1.930 389	1.942 696	1.942 696	1.985 002	1.985 002

with mixed BC through the relation

$$2(E_{q;i}(2N+1)-E_{-1/2;0}(2N+1))=E_j(N)-E_0(N). \tag{21}$$

Here, $E_j(N)$ are the energy levels for mixed BC. This relation was checked for the Ising and three-state Potts models.

It is a curious fact that the sectors which are formally singled out by (14) due to the modulo condition (cf (9) and (11)) would also allow a finite-size projection mechanism. For example, consider for $m=5$ the sectors $\mathscr{E}_{-5/2}(2N+1)$ and $\mathscr{E}_{7/2}(2N+1)$ where the latter is completely contained in the former. However, this would yield heighest weights Δ not contained in the discrete series of (7).

A projection mechanism like that one described above also works for toroidal BC (Alcaraz *et al* 1989). This is a numerical observation and we have no mathematical proof for it. The same projection procedure (for a finite number of sites) does not work in this simple form for the other three classes of models (see table 1). However, we assume that similar phenomena should occur in higher-spin Hamiltonians with O(2) symmetry (di Francesco *et al* 1988).

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