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Operator content of the Ising model with three-spin coupling

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Abstract. The Ising quantum-chain with staggered three-spin coupling is studied for free and torodial boundary conditions. The operator content of the finite-size limit of the spectra is conjectured. It is found to be related to the operator content of the Ashkin-Teller model.

The Ising quantum chain with $3N$ sites with staggered three-spin coupling is defined by (Alcaraz and Barber 1987)

$$H=-\frac{1}{\mathcal{N}}\sum_{i=0}^{N-1}\{\sigma_{3i}^{x}\sigma_{3i+1}^{x}\sigma_{3i+2}^{x}+\varepsilon\sigma_{3i+1}^{x}\sigma_{3i+2}^{x}\sigma_{3i+3}^{x}+\varepsilon\sigma_{3i+2}^{x}\sigma_{3i+3}^{x}\sigma_{3i+4}^{x}$$
$$+\lambda(\varepsilon\sigma_{3i}^{z}+\sigma_{3i+1}^{z}+\varepsilon\sigma_{3i+2}^{z})\}. \qquad (1)$$

σ^x and σ^z are Pauli matrices, ε is the coupling constant, λ plays the role of an inverse temperature. The model is self-dual and has a second-order phase transition at $\lambda=1$ for $0<|\varepsilon|\leqslant 1$ corresponding to a Virasoro algebra with $c=1$. $\mathcal{N}$ is a constant which has to be chosen such that H is conformally invariant (see below). By numerical studies of H with periodic and free boundary conditions (BC), Alcaraz and Barber (1987) and Iglói (1988) found exponents occurring in the Ashkin-Teller (AT) model (Ashkin and Teller 1943, Baake *et al* 1987a, b).

The aim of this paper is to give a conjecture of the operator content for free and toroidal BC and to verify it numerically. For this purpose H was diagonalised for chains up to 19 (free BC), respectively 21 (toroidal BC) sites for the domain $-1\leqslant\varepsilon\leqslant 1$. The spectra are found to be the same for $-\varepsilon$ and ε. The conjectured operators are identical to those of the AT model for *positive* ε. For $\varepsilon=0$ the three-spin model has a trivial solution, whereas the AT model decouples into two independent Ising models.

This paper is organised as follows. First we define the various BC and discuss the symmetries of the three-spin model. After a short review of the symmetries of the AT model we give the conjectured operator content of the three-spin model and discuss the relations to the AT model.

We first consider toroidal boundary conditions. Because of the staggered coupling, the situation is different for $3N$ and $3N+p$ sites ($p=1,2$).

Periodic boundary conditions for chains with $3N$ sites (1) are defined by $\sigma_{3N}^{x}=\sigma_{0}^{x}$ and $\sigma_{3N+1}^{x}=\sigma_{1}^{x}$. The resulting Hamiltonian (denoted by H_{3N}) has a $\mathbf{Z}_2\otimes\mathbf{Z}_2$ symmetry generated by the 'charge' operators

$$P_0=\prod_{i=0}^{N-1}\sigma_{3i}^{z}\sigma_{3i+1}^{z}\qquad P_2=\prod_{i=0}^{N-1}\sigma_{3i+1}^{z}\sigma_{3i+2}^{z}. \qquad (2)$$

This group allows us to decompose the spectra of H_{3N} into sectors labelled by the eigenvalues of P_0 and P_2.

H_{3N}, P_0 and P_2 are invariant under translation of three steps:

$$T: \sigma_i \to \sigma_{i+3} \qquad \sigma \in \{\sigma^x, \sigma^z\}. \tag{3}$$

This operation has been used to prediagonalise H_{3N} into sectors with different momenta $K \in \{0 \ldots N-1\}$ defined by the eigenvalues of $T = \exp[(2\pi i/N)K]$.

H_{3N} also commutes with the reflection

$$S: \sigma_i \to \sigma_{3N-1-i}. \tag{4}$$

S and T obey $ST = T^{-1}S$ and thus span $\mathbf{D}_N$. S does not commute with the charges:

$$SP_0 = P_2 S \tag{5}$$

it allows us to split the sectors with momentum zero and charges ++ (i.e. $P_0 = +1$, $P_2 = +1$) and −−.

Because of (5), the 'inner' and the 'dynamical' symmetry ($\mathbf{Z}_2 \otimes \mathbf{Z}_2$ and $\mathbf{D}_N$) are not independent. The total symmetry group G is a *semi*direct product of $\mathbf{Z}_2 \otimes \mathbf{Z}_2$ and $\mathbf{D}_N$:

$$\mathrm{G} = (\mathbf{Z}_2 \otimes \mathbf{Z}_2) \otimes_s \mathbf{D}_N \tag{6}$$

where $\mathbf{Z}_2 \otimes \mathbf{Z}_2$ is normal in G.

The $\mathbf{Z}_2 \otimes \mathbf{Z}_2$ allows one to define four toroidal boundary conditions for H_{3N}:

BC	σ^x_{3N}	σ^x_{3N+1}
++	σ^x_0	σ^x_1
−+	$-\sigma^x_0$	$-\sigma^x_1$
+−	σ^x_0	$-\sigma^x_1$
−−	$-\sigma^x_0$	σ^x_1.

The resulting Hamiltonians are denoted by H^{ab}_{3N} for BC ab, ($a, b \in \{+, -\}$, $H_{3N} \equiv H^{++}_{3N}$). They all have the $\mathbf{Z}_2 \otimes \mathbf{Z}_2$ symmetry and are invariant under the modified translation

$$\bar{T} = B_{ab} T \tag{7}$$

where B_{ab} depends on the BC ab and acts on the first three sites of a chain:

$$B_{++} = 1 \qquad B_{-+} = \sigma^x_0 \sigma^x_1 \qquad B_{+-} = \sigma^x_1 \sigma^x_2 \qquad B_{--} = \sigma^x_0 \sigma^x_2. \tag{8}$$

$\bar{T}$, P_0 and P_2 commute and have been used to prediagonalise the Hamiltonians H^{ab}_{3N}.

The symmetry is larger for $\varepsilon = 1$. Since there is no staggered coupling at this point, H_{3N} is additionally invariant under translation of *one* step

$$t: \sigma_i \to \sigma_{i+1}. \tag{9}$$

t does not commute with the charges:

$$P_0 t = t P_2 \qquad P_2 t = t P_0 P_2. \tag{10}$$

P_0, P_2, t and S span a semidirect product of $\mathbf{Z}_2 \otimes \mathbf{Z}_2$ with $\mathbf{D}_{3N}$

$$\mathrm{G}_1 = (\mathbf{Z}_2 \otimes \mathbf{Z}_2) \otimes_s \mathbf{D}_{3N}. \tag{11}$$

Again the inner and dynamical symmetries are not independent.

We now consider the case of $3N+p$ sites ($p = 1, 2$). We define periodic BC for (1) by changing the sum $\Sigma_{i=0}^{N-1}$ to $\Sigma_{i=0}^{N}$ and choosing $\sigma^x_{3N+p} = \sigma^x_0$, $\sigma^x_{3N+p+1} = \sigma^x_1$ and $\sigma^x_i = \sigma^z_i = 0$ for $i > 3N+p+1$. The resulting Hamiltonian is denoted by H_{3N+p}.

For $\varepsilon \neq 1$ there is no invariance under translation or reflection. Furthermore, there are no conserved charges similar to P_0 and P_2. At the point $\varepsilon = 1$ H_{3N+p} commutes with t and S (here: $S: \sigma_i \to \sigma_{3N+p-1-i}$). As will be seen later, H_{3N+p} with $\varepsilon = 1$ can be interpreted as an additional toroidal BC related to the higher symmetry of H_{3N} at $\varepsilon = 1$. In this paper we only consider this value of the coupling constant. The case $\varepsilon \neq 1$ is currently being investigated.

The staggered coupling allows us to define three types of free boundary conditions for (1) (Iglói 1987). A Hamiltonian H^f_{3N+p} of type f with $3N+p$ sites ($p, f \in \{0, 1, 2\}$) is defined by

$$H^f_{3N+p} = -\frac{1}{\mathcal{N}} \sum_{i=0}^{N} \{\sigma^x_{3i}\sigma^x_{3i+1}\sigma^x_{3i+2} + \varepsilon\sigma^x_{3i+1}\sigma^x_{3i+2}\sigma^x_{3i+3} + \varepsilon\sigma^x_{3i+2}\sigma^x_{3i+3}\sigma^x_{3i+4} + \lambda(\varepsilon\sigma^z_{3i} + \sigma^z_{3i+1} + \varepsilon\sigma^z_{3i+2})\} \tag{12}$$

where

$$\sigma^x_j = \sigma^z_j = 0 \qquad \begin{cases} \text{for } j > 3N+p-1 & \text{for type } f = 0 \\ \text{for } j > 3N+p \text{ and } j = 0 & \text{for type } f = 1 \\ \text{for } j > 3N+p+1 \text{ and } j = 0, 1 & \text{for type } f = 2. \end{cases} \tag{13}$$

H^f_{3N+p} commutes with the charge operators defined analogous to (2) for *each* number of sites:

$$P_0 = \prod_{i=0}^{N} \sigma^z_{3i}\sigma^z_{3i+1} \qquad P_2 = \prod_{i=0}^{N} \sigma^z_{3i+1}\sigma^z_{3i+2}. \tag{14}$$

with $\sigma^z_j = 1$ for undefined j (see (13)).

The behaviour under reflection $S: \sigma_i \to \sigma_{3N+p-1-i}$ depends on the type f. A chain with $3N+p$ sites and type $f = p$ is invariant, whereas the two other types $f \neq p$ are mapped to each other:

$$H^p_{3N+p}S = SH^p_{3N+p} \qquad H^{p+1}_{3N+p}S = SH^{p+2}_{3N+p}. \tag{15}$$

The charges are mapped according to

$$SP_0 = P_2S. \tag{16}$$

Because of (15) and (16), only seven of the twelve charge sectors of the three types of chains are independent.

The connection between the different types and the operators P_0, P_2 and S can be understood in the following way. Let $\tilde{t}$ be the operation which increases the type f by one:

$$\tilde{t}H^f_{3N+p} = H^{f+1}_{3N+p}\tilde{t} \qquad \tilde{t}^3 = 1 \tag{17}$$

which is something like a translation of the chain on the 'grid' of the staggered coupling constants. For $\varepsilon = 1$ the three types are identical, and H^f_{3N+p} commutes with $\tilde{t}$ for each f and p. $\tilde{t}$ obeys

$$P_0\tilde{t} = \tilde{t}P_2 \qquad P_2\tilde{t} = \tilde{t}P_0P_2 \qquad S\tilde{t} = \tilde{t}^{-1}S. \tag{18}$$

Thus P_0, P_2, S and $\tilde{t}$ span $(\mathbf{Z}_2 \otimes \mathbf{Z}_2) \otimes_s \mathbf{D}_3$ which is isomorphic to a subgroup of G_1 (11). So the existence of the three types of free BC can be understood as a consequence of the additional $\mathbf{Z}_3$ symmetry of the system at the point $\varepsilon = 1$.

After this discussion of the symmetries for the three-spin model, we give a review of the situation for the AT model. For details we refer to Baake *et al* (1987a, b).

The AT model consists of two commuting Ising models coupled through a parameter ε. The total symmetry group for a quantum chain with N sites and periodic BC is a direct product of the inner symmetry group $\mathbf{D}_4=\{C^i\Sigma^j \mid i=0,1;\ j=0,1,2,3;\ C^2=1;\ \Sigma^4=1;\ C\Sigma=\Sigma^{-1}C\}$ with the dynamical symmetry group $\mathbf{D}_N$ spanned by reflection (or 'parity') and translation. For $\varepsilon=1$ the model is identical to the four-state Potts model (Potts 1952). Here the inner symmetry increases to $\mathbf{S}_4\equiv\mathbf{D}_4\otimes_s\mathbf{Z}_3=\{\Omega^iC^j\Sigma^k \mid i=0,1,2; j=0,1;\ k=0,1,2,3\}$.

The $\mathbf{D}_4$ allows us to define five classes of toroidal BC:

$$\text{I: } 1 \qquad \text{II: } \Sigma^2 \qquad \text{III: } C\Sigma, C\Sigma^3 \qquad \text{IV: } C\Sigma^2 \qquad \text{V: } \Sigma, \Sigma^3.$$

The larger symmetry $\mathbf{S}_4$ at the Potts point $\varepsilon=1$ allows us to define a class of BC which contains no elements of $\mathbf{D}_4$ (Grimm 1988). This class is represented by an element $\Omega\in\mathbf{S}_4$ of order three.

We now turn to determining the operator content of the three-spin model for toroidal boundary conditions.

The quantities

$$\mathscr{E}^{ab,cd}_{K^S,i}(\varepsilon)=\lim_{N\to\infty}\frac{3N}{2\pi}\left(E^{ab,cd}_{K^S,i}(\varepsilon,3N)-E^{++,++}_{0^+,1}(|\varepsilon|,3N)\right) \tag{19}$$

define the finite-size spectrum (Cardy 1984, 1986, von Gehlen and Rittenberg 1986), where $E^{ab,cd}_{K^S,i}(\varepsilon,3N)$ is the ith energy level of H^{ab}_{3N} with momentum K, charges cd and $3N$ sites. S labels the sectors with S decomposition. Note that the gaps $\mathscr{E}^{ab,cd}_{K^S,i}(\varepsilon)$ are defined relative to the groundstate $E^{++,++}_{0^+,1}(|\varepsilon|,3N)$ with *positive* coupling constant $|\varepsilon|$. The extrapolation $N\to\infty$ has been done with the algorithm of Bulirsch and Stoer (1964), (see also Henkel and Schütz 1988).

It is a consequence of conformal invariance in two dimensions that the $\mathscr{E}^{ab,cd}_{K^S,i}(\varepsilon)$ can be described in terms of irreducible representations (irreps) of two commuting Virasoro algebras L_n, $\bar{L}_n$ with central charge $c=1$:

$$[L_n,L_m]=(n-m)L_{n+m}+\tfrac{1}{12}cn(n^2-1)\delta_{n,-m} \qquad n,m\in\mathbf{Z}. \tag{20}$$

An irrep $(\Delta,\bar{\Delta})$ characterised by the highest weights Δ and $\bar{\Delta}$

$$\begin{aligned} &L_0|\Delta,\bar{\Delta}\rangle=\Delta|\Delta,\bar{\Delta}\rangle\\ &\bar{L}_0|\Delta,\bar{\Delta}\rangle=\bar{\Delta}|\Delta,\bar{\Delta}\rangle\\ &\bar{L}_n|\Delta,\bar{\Delta}\rangle=L_n|\Delta,\bar{\Delta}\rangle=0 \qquad n>0 \end{aligned} \tag{21}$$

generates a level

$$\mathscr{E}_K=(\Delta+r)+(\bar{\Delta}+\bar{r}) \tag{22}$$

with momentum

$$K=(\Delta+r)-(\bar{\Delta}+\bar{r}) \tag{23}$$

and degeneracy $d(\Delta,r)d(\bar{\Delta},\bar{r})$, r, $\bar{r}\in\mathbf{N}_0$.

For $c=1$ $d(\Delta,r)$ is independent of Δ and equal to the function $\pi(r)$ determined by the partition function

$$\pi_v(q)=\prod_{m=1}^{\infty}\frac{1}{1-q^m}=\sum_{r=0}^{\infty}\pi(r)q^r \tag{24}$$

unless $\Delta = t^2/4$, where t is an integer. In this case $d(\frac{1}{4}t^2, t)$ is determined by the partition function (Kac 1979)

$$(1-q^{t+1})\pi_v(q) = \sum_{r=0}^{\infty} d(\tfrac{1}{4}t^2, r)q^r. \tag{25}$$

The factor $\mathcal{N}$ of the Hamiltonian H has been chosen such that

$$\lim_{N\to\infty} \frac{3N}{2\pi}(E_{1,1}^{++,+-}(\varepsilon, 3N) - E_{0,1}^{++,+-}(\varepsilon, 3N)) = 1. \tag{26}$$

(von Gehlen *et al* 1985). The data for $\mathcal{N}$ are listed in table 1.

Table 1. Normalisation factor $\mathcal{N}$ of Hamiltonian (1).

ε	$\mathcal{N}$
0.01	0.0424
0.1	0.4214
0.2	0.8282
0.4	1.569
0.5	1.901
0.8	2.760
1.0	3.224

The $E_{K^S,i}^{ab,cd}(\varepsilon, 3N)$ have been computed for chains of up to 21 sites. The following sectors are found to be identical:

$$E_{K,i}^{ab,cd}(\varepsilon, 3N) = E_{K,i}^{ba,dc}(\varepsilon, 3N) = E_{K,i}^{cd,ab}(\varepsilon, 3N) \tag{27}$$

with a, b, c, $d \in \{+, -\}$. Thus only seven of the sixteen charge sectors for the four BC are independent.

As mentioned above, the spectra are identical for positive and negative coupling constants. The mapping is as follows:

$$E_{K,i}^{ab,cd}(-\varepsilon, 3N) = E_{K,i}^{ab,cd}(\varepsilon, 3N) \qquad N \text{ even} \tag{28}$$

for each a, b, c, $d \in \{+, -\}$, $K \in N_0$ and $\varepsilon > 0$.

$$\left.\begin{aligned}
E_{K,i}^{++,++}(-\varepsilon, 3N) &= E_{K,i}^{--,--}(\varepsilon, 3N)\\
E_{K,i}^{--,--}(-\varepsilon, 3N) &= E_{K,i}^{++,++}(\varepsilon, 3N)\\
E_{\tilde{K},i}^{--,+-}(-\varepsilon, 3N) &= E_{K,i}^{++,+-}(\varepsilon, 3N)\\
E_{\tilde{K},i}^{++,+-}(-\varepsilon, 3N) &= E_{K,i}^{--,+-}(\varepsilon, 3N)\\
E_{K^S,i}^{++,--}(-\varepsilon, 3N) &= E_{K^S,i}^{++,--}(\varepsilon, 3N)\\
E_{K,i}^{+-,+-}(-\varepsilon, 3N) &= E_{K,i}^{+-,+-}(\varepsilon, 3N)\\
E_{K,i}^{+-,-+}(-\varepsilon, 3N) &= E_{K,i}^{+-,-+}(\varepsilon, 3N)
\end{aligned}\right\} \quad N \text{ odd} \tag{29}$$

for each $\varepsilon > 0$, $K \in \mathrm{N}_0$ and $S \in \{+, -\}$ where $\tilde{K} = (N/2 - K) \bmod N$.

Because of the occurrence of antiferromagnetic waves, the momenta $\tilde{K}$ of $E_{\tilde{K},i}^{--,+-}(-\varepsilon, 3N)$ and $E_{\tilde{K},i}^{++,+-}(-\varepsilon, 3N)$ defined through $\tilde{T} = \exp[(2\pi i/N)\tilde{K}]$ are not identical to the momenta K defined in (23).

The finite-size scaling spectra $\mathscr{E}^{ab,cd}_{K^{S},i}(\varepsilon)$ can be described in terms of sectors of the AT model. We use the notation of Baake *et al* (1987a, b) and define two sectors.

(a) Sectors with integer momentum K

$$\begin{aligned}
&\mathscr{A}=(\{0\},\{0\})\oplus(\{1\},\{1\})\oplus\mathscr{A}_1\\
&\mathscr{B}=(\{0\},\{1\})\oplus(\{1\},\{0\})\oplus\mathscr{A}_1\\
&\mathscr{A}_1=\bigoplus_{n\geqslant 0}\left(((n+1)^2h,(n+1)^2h)\oplus\left(\frac{(n+1)^2}{2},\frac{(n+1)^2}{2}\right)\right)\\
&\qquad\oplus R(4,4;4,4|h)\oplus R(4,4;-4,-4|h)\\
&\mathscr{C}=R(4,2;4,2|h)\oplus R(4,4;-4,-2|h)\\
&\mathscr{E}=\bigoplus_{n\geqslant 0}\left(\frac{(2n+1)^2}{16h},\frac{(2n+1)^2}{16h}\right)\oplus R(2,1;4,4|h)\oplus R(-2,-1;4,4|h)\\
&\mathscr{F}=\bigoplus_{n\geqslant 0}\left(\frac{(2n+1)^2}{4h},\frac{(2n+1)^2}{4h}\right)\oplus R(4,2;4,4|h)\oplus R(4,2;-4,-4|h)\\
&\mathscr{G}=\mathscr{F}\left(\frac{1}{h}\right)\\
&\mathscr{H}=([\tfrac{1}{16}]_1,[\tfrac{1}{16}]_1)\oplus([\tfrac{9}{16}]_1,[\tfrac{9}{16}]_1).
\end{aligned}\tag{30}$$

(b) Sectors with half-integer momentum K

$$\begin{aligned}
&\mathscr{I}=R(4,2;2,1|h)\oplus R(4,2;-2,-1|h)\\
&\mathscr{J}=\mathscr{I}(1/h)\\
&\mathscr{K}=([\tfrac{9}{16}]_1,[\tfrac{1}{16}]_1)\oplus([\tfrac{1}{16}]_1,[\tfrac{9}{16}]_1)
\end{aligned}\tag{31}$$

where

$$\begin{aligned}
&R(p,q;r,s|h)=\bigoplus_{m\geqslant 0,n\geqslant 0}\left(\frac{(pm+q+(rn+s)h)^2}{16h},\frac{(pm+q-(rn+s)h)^2}{16h}\right)\\
&\{0\}=\bigoplus_{k\geqslant 0}(4k^2)\\
&\{1\}=\bigoplus_{k\geqslant 0}((2k+1)^2)\\
&[\tfrac{1}{16}]_1=\bigoplus_{k\in\mathbf{Z}}[\tfrac{1}{16}(8k+1)^2]\\
&[\tfrac{9}{16}]_1=\bigoplus_{k\in\mathbf{Z}}[\tfrac{1}{16}(8k+3)^2]
\end{aligned}\tag{32}$$

and (Δ) is an irrep of the Virasoro algebra (20) with highest weight Δ (see equation (21)). Since the operator content depends on $|\varepsilon|$, we define

$$h=\frac{\pi}{4\cos^{-1}(-|\varepsilon|)}.\tag{33}$$

Table 2 shows the conjectured operator content. It has been verified numerically. Table 3 illustrates a part of the data.

Comparing these results with the AT model, we observe that the operator content is the same if we identify the charges P_0 and P_2 with the elements $C\Sigma^3$ and $C\Sigma$ of the AT $\mathbf{D}_4$. $C\Sigma^3$ and $C\Sigma$ generate a $\mathbf{Z}_2\otimes\mathbf{Z}_2$ subgroup of $\mathbf{D}_4$. Furthermore G (6) and G_1

Table 2. Conjectured operator content for toroidal BC.

BC	P_0P_2	Operator content
++	++	$\mathscr{A}+\mathscr{F}$
	−−	$\mathscr{C}+\mathscr{G}$
	+−	$\mathscr{H}$
−−	−−	$\mathscr{B}+\mathscr{F}$
	+−	$\mathscr{K}$
−+	+−	$\mathscr{J}$
	−+	$\mathscr{E}$

(11) can be understood as subgroups of the AT symmetry groups $\mathbf{D}_4 \otimes \mathbf{D}_N$ and $\mathbf{S}_4 \otimes \mathbf{D}_N$. No operator has been found yet which corresponds to $C \in \mathbf{D}_4$. Note that the reflection S is not equivalent to C because it is not a local operator, i.e. it does not commute with the translation T. Because of the lack of 'C' operation for the three-spin model, only those BC are realised which are equivalent to the AT BC I, II and III.

We now present the results for chains with $3n+p$ sites ($p=1,2$) and periodic BC. The quantities

$$\mathscr{E}_i^p = \lim_{N\to\infty} \frac{3N+p}{2\pi}(E_i(3N+p) - E_0(3N+p)) \tag{34}$$

define the finite size spectrum. As mentioned above, we only consider the case $\varepsilon = 1$. $E_i(3N+p)$ is the ith eigenvalue of H_{3N+p}. The reference energies $E_0(3N+p)$ have been calculated by interpolating the ground-state energies $E_{0^+,1}^{++;++}(\varepsilon=1, 3N)$ with polynominals such that $E_0(3N) = E_{0^+,1}^{++;++}(\varepsilon = 1, 3N)$.

The extrapolation has been done for fixed p and chains of up to 17 sites. We observed $\mathscr{E}_i^1 = \mathscr{E}_i^2$. The $\mathscr{E}_i^p$ are found to be identical with the lower part of the operator content of the AT model with Ω BC at the Potts point $\varepsilon = 1$. This is given by (Grimm 1988):

$$((\langle\tfrac{1}{6}\rangle, \langle\tfrac{1}{6}\rangle) \oplus (\langle\tfrac{1}{3}\rangle, \langle\tfrac{1}{3}\rangle) \tag{35}$$

where

$$\langle\tfrac{1}{6}\rangle = \bigoplus_{m\in\mathbf{Z}} ((m+\tfrac{1}{6})^2) \qquad \langle\tfrac{1}{3}\rangle = \bigoplus_{m\in\mathbf{Z}} ((m+\tfrac{1}{3})^2).$$

Thus the chain with $3N+p$ ($p=1,2$) sites can be understood as an additional BC caused by the higher symmetry at $\varepsilon = 1$.

We turn now to determining the operator content for free boundary conditions. The quantities

$$\mathscr{E}_i^{ab,f,p} = \lim_{N\to\infty} \frac{3N+p}{\pi}(E_i^{ab,f}(3N+p) - E_1^{++,f}(3N+p)) \tag{36}$$

define the finite size spectrum (Cardy 1984, 1986, von Gehlen and Rittenberg 1986) for a fixed type f. $E_i^{ab,f}(3N+p)$ is the ith eigenvalue of H_{3N+p}^f in the charge sector ab. The spectrum has been calculated for chains up to 19 sites. It is identical for positive and negative ε for each a, b, f and p.

The spectra $\mathscr{E}_i^{ab,f,p}$ are generated by unitary irreps of one Virasoro algebra (20). An irrep characterised by the highest weight Δ

$$L_0|\Delta\rangle = \Delta|\Delta\rangle \tag{37}$$

Table 3. Extrapolated levels $\mathscr{E}^{ab,cd}_{K\ s,i}$ (equation (19)) for toroidal, non-periodic BC and $\varepsilon = 0.2$.

BC	P_0P_2	K	Theoretical $\Delta+\bar{\Delta}+r+\bar{r}$	d	Extrapolated
$--$	$+-$	$\frac{1}{2}$	0.625	1	0.6250 (2)
		$\frac{1}{2}$	0.625+1+1	1	2.623 (6)
		$\frac{3}{2}$	0.625+1+0	1	1.625 (2)
		$\frac{3}{2}$	0.625+2+1	2	3.5 (2) 3.6 (1)
		$\frac{1}{2}$	1.625+0+1	1	2.620 (5)
		$\frac{1}{2}$	1.625+2+0	2	3.6 (1) 3.61 (7)
$+-$	$+-$	$\frac{1}{2}$	0.503 64	1	0.5039 (2)
		$\frac{1}{2}$	0.503 64+1+1	1	2.50 (1)
		$\frac{3}{2}$	0.503 64+1+0	1	1.501 (6)
		$\frac{3}{2}$	0.503 64+2+1	2	3.44 (5) 3.50 (1)
		$\frac{1}{2}$	0.500 96+1+0	1	1.504 (1)
		$\frac{1}{2}$	0.500 96+2+1	2	3.4 (2) 3.4 (2)
		$\frac{3}{2}$	0.500 96+2+0	2	2.43 (3) 2.43 (1)
		$\frac{3}{2}$	2.276 39	1	2.25 (1)
		$\frac{1}{2}$	2.276 39+0+1	1	3.2 (1)
		$\frac{3}{2}$	2.760 02	1	2.763 (4)
		$\frac{1}{2}$	2.760 02+0+1	1	3.7 (2)
$--$	$--$	0	0.886 38	1	0.8815 (1)
		0	0.886 38+1+1	1	2.8 (1)
		1	0.886 38+1+0	1	1.879 (5)
		1	0.886 38+2+1	2	3.7 (4) 3.86 (3)
		2	0.886 38+2+0	2	2.7 (1) 2.81 (2)
		0	1.128 19	1	1.1342 (5)
		0	1.128 19+1+1	1	3.1(1)
		1	1.128 19+1+0	1	2.130 (5)
		1	1.128 19+2+1	2	3.9 (2) —
		2	1.128 19+2+0	2	3.05 (5) 3.04 (4)
		0	3.545 51	1	3.49 (4)
		1	1	1	1.000 (1)
		0	1+1+2	1	3.8 (1)
		2	1+1+0	1	1.91 (2)
		0	1+2+1	1	4.00 (2)
		1	1+2+0	1	3.02 (1)
		2	2.014 56	1	2.01 (1)
		1	2.014 56+0+1	1	2.97 (2)
$+-$	$-+$	0	0.282 05	1	0.26638 (4)
		0	0.282 05+1+1	1	2.23 (3)
		1	0.282 05+1+0	1	1.285 (2)
		1	0.282 05+2+1	2	3.11 (6) 3.09 (1)
		2	0.282 05+2+0	2	2.27 (4) 2.23 (1)
		1	1.168 42	1	1.165 (1)
		1	1.168 42+1+1	1	3.1 (1)
		2	1.168 42+1+0	1	2.14 (4)
		2	1.168 42+2+1	2	3.9 (1) 3.7 (2)
		0	1.168 42+1+0	1	2.165 (2)
		0	1.168 42+2+1	2	4.2 (2) —
		1	1.168 42+2+0	2	3.07 (1) —
		0	2.538 42	1	2.55 (1)

Table 4. Conjectured operator content for free BC.

p	f	Charges	Operator content
0	0	$++$	$D_{0,0}+\tilde{D}$
		$--$	$D_{0,1}+\tilde{D}$
		$+-$	D
	1	$++$	$D_{0,0}+D$
		$--$	D
		$+-$	D
		$-+$	$D_{0,1}+\tilde{D}$
1	1	$++$	$D_{0,0}+\tilde{D}$
		$--$	$D_{0,1}+\tilde{D}$
		$+-$	D
	0	$++$	$D_{0,0}+\tilde{D}$
		$--$	D
		$+-$	$D_{0,1}+\tilde{D}$
		$-+$	D
2	2	$++$	$D_{0,0}+\tilde{D}$
		$--$	$D_{0,1}+\tilde{D}$
		$+-$	D
	0	$++$	$D_{0,0}+\tilde{D}$
		$--$	D
		$+-$	D
		$-+$	$D_{0,1}+\tilde{D}$

gives a contribution

$$\mathscr{E}_r=\Delta+r \tag{38}$$

to the spectra $\mathscr{E}_i^{f,p}$. Δ is a surface critical exponent and the level $|\Delta+r\rangle$ has a degeneracy $d(\Delta, r)$ (24), (25) and a relative parity $(-1)^r$ to the level $|\Delta\rangle$.

All conjectured levels $\mathscr{E}_i^{ab,f,p}$ are identical with the lower part of the AT sectors found by Baake *et al* (1987a). They defined

$$\begin{aligned}
D_{0,0}&=\bigoplus_{k\geq 0}(4k^2)^+\oplus\bigoplus_{k\geq 1}\left(\frac{4k^2}{h}\right)^+\\
D_{0,1}&=\bigoplus_{k\geq 0}((2k+1)^2)^+\oplus\bigoplus_{k\geq 1}\left(\frac{4k^2}{h}\right)^-\\
\tilde{D}&=D_{1,0}=D_{1,1}=\bigoplus_{k\geq 0}\left(\frac{(2k+1)^2}{h}\right)^+\\
D&=\bigoplus_{k\geq 0}\left(\frac{(2k+1)^2}{4h}\right)^+.
\end{aligned} \tag{39}$$

(The parities in (39) are always defined relative to the lowest level within each sector which is taken, by convention, to have parity $+$.)

Table 4 shows the conjectured operator content.

These results lead us to the following conjectures.

(i) For $f=p$ we can identify AT and three-spin sectors choosing $P_0=C\Sigma^3$ and $P_2=C\Sigma$ as for toroidal BC (18).

(ii) The operator content is identical for each p and f (cf Iglói 1987) where the charge sectors are mapped according to (15)-(18).

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