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LETTER TO THE EDITOR

The spectra of quantum chains with free boundary conditions and Virasoro algebras

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Abstract. At the critical point the spectra of quantum chains with periodic and twisted boundary conditions are described by irreducible representations of two Virasoro algebras with the same central charge. We show that in the case of free boundary conditions, the spectra can be understood in terms of irreducible representations of a single Virasoro algebra. For the Ising and the three-state Potts models, the corresponding irreducible representations are identified.

Using conformal invariance (Cardy 1986a and references therein) in a recent paper we have determined numerically the finite-size limit of the spectra of the three-state Potts quantum chain (von Gehlen and Rittenberg 1986b). Periodic and twisted boundary conditions have been used and it has been shown that the spectra can be described in terms of a few irreducible representations of two commuting Virasoro algebras. In this way *all* the bulk critical exponents have been determined. In the present letter we consider the spectra of quantum chains with free boundary conditions with the aim of determining *all* the surface critical exponents.

We consider first the two-point correlation function in a half plane ($-\infty<x<\infty$, $y\geq 0$) with free boundary conditions. If we are at the critical point and the operator φ has scaling dimensions x, it was shown by Cardy (1984) using conformal invariance that the correlation function has the form

$$\langle\varphi(x_1, y_1)\varphi(x_2, y_2)\rangle=(y_1y_2)^{-x}F(\rho) \tag{1}$$

where

$$\rho=\frac{y_1y_2}{(x_1-x_2)^2+(y_1-y_2)^2}. \tag{2}$$

The function $F(\rho)$ depends on the operator φ which appears in the correlation function and has the following asymptotic behaviours:

$$\underset{\rho\to 0}{F(\rho)}=\rho^{x_s}R(\rho) \qquad \underset{\rho\to\infty}{F(\rho)}\sim\rho^{x} \tag{3}$$

where the function $R(\rho)$ is regular at $\rho=0$ and x_s is the surface exponent (Binder 1983, Cardy 1986a). We now perform the conformal transformation

$$w=(N/\pi)\ln z=(N/\pi)\ln(x+\mathrm{i}y)=\tau+\mathrm{i}v \tag{4}$$

which maps the half plane on the strip ($-\infty<\tau<\infty$, $-\frac{1}{2}N\leq v\leq\frac{1}{2}N$). Here τ can be interpreted as the Euclidean time. The correlation function on the strip is

$$\langle\varphi(v_1, \tau_1)\varphi(v_2, \tau_2)\rangle$$

$$= \left(\frac{\pi}{N}\right)^{2x} |z_1 z_2|^x \rho^{x_s} R(\rho)$$

$$= \left(\frac{\pi}{N}\right)^{2x} \left(\sin\frac{\pi}{N}v_1 \sin\frac{\pi}{N}v_2\right)^{x_s - x} \sum_{r=0}^{\infty} a_r(v_1, v_2)$$

$$\times \exp[-(\pi/N)(x_s + r)(\tau_2 - \tau_1)] \tag{5}$$

where a_0 is independent of v_1 and v_2. Assume now that the Euclidean time evolution of the system is described by a Hamiltonian H with eigenvalues $E^{(F)}(r)(E^{(F)} < E^{(F)}(0) < E^{(F)}(1) < \ldots)$:

$$H|r\rangle = E^{(F)}(r)|r\rangle \tag{6}$$

$E^{(F)}$ being the ground state energy. Using the standard spectral decomposition, the correlation function of (5) can be re-expressed as follows:

$$\langle\varphi(v_1, \tau_1)\varphi(v_2, \tau_2)\rangle$$

$$= \sum_{r=0}^{\infty} \exp[-(E^{(F)}(r) - E^{(F)})(\tau_2 - \tau_1)]\langle 0|\varphi(0, v_1)|r\rangle\langle r|\varphi(0, v_2)|0\rangle. \tag{7}$$

In the sum over the r one has to keep in mind that several states can correspond to the same energy level $E^{(F)}(r)$.

Comparing (5) and (6) we notice the relation

$$(N/\pi)(E^{(F)}(r) - E^{(F)}) = x_s + r \qquad (r = 0, 1, \ldots). \tag{8}$$

We now recall that the known surface exponents x_s coincide with lowest weights Δ of irreducible representations of the Virasoro algebra with the central charge c fixed by the universality class (Cardy 1984, von Gehlen and Rittenberg 1986a). The relation (8) then suggests that the finite-size limit of the spectrum of the Hamiltonian with free boundary conditions is given by the lowest weight and the descendents of irreducible representations of the Virasoro algebra. The degeneracy of the level $(\Delta + r)$ that we denote by $d(\Delta, r)$ can be computed using the character formula of Rocha-Caridi (1985). It is important to notice that in the case of periodic or twisted boundary conditions the spectrum in the finite-size limit is given by a pair of irreducible representations $(\Delta, \bar{\Delta})$ corresponding to two Virasoro algebras and has a much richer structure (Cardy 1986b, von Gehlen and Rittenberg 1986b, Henkel 1986).

Table 1. The degeneracy $d(\Delta, r)$ for the irreducible representation Δ and the descendent r for the Ising model.

	r										
Δ	0	1	2	3	4	5	6	7	8	9	10
0	1	0	1	1	2	2	3	3	5	5	7
$\frac{1}{2}$	1	1	1	1	2	2	3	4	5	6	8
$\frac{1}{16}$	1	1	1	1	2	3	4	5	6	8	10

In order to check these ideas we consider the Ising and the three-state Potts quantum chains. We start with the Ising model which is defined by the Hamiltonian

$$H^{(F)}=-\tfrac{1}{2}\sum_{i=1}^{N}(\sigma_i+\lambda\Gamma_i\Gamma_{i+1})\qquad(\Gamma_{N+1}=0)\tag{9a}$$

where

$$\sigma=\begin{pmatrix}1&0\\0&-1\end{pmatrix}\qquad\Gamma=\begin{pmatrix}0&1\\1&0\end{pmatrix}\tag{9b}$$

and N indicates the number of sites. This Hamiltonian can be diagonalised exactly (Boccara and Sarma 1974, Burkhardt and Guim 1985); at the critical point $\lambda=1$ it has the form

$$H^{(F)}=\sum_{n=0}^{N-1}\frac{n+\frac{1}{2}}{N+\frac{1}{2}}\pi(a_n^+a_n+\tfrac{1}{2})\tag{10}$$

where $a_n(a_n^+)$ are fermionic annihilation (creation) operators. Since the Ising model has Z_2 symmetry, we consider separately the charge-zero spectrum (even number of fermions) $E_0^{(F)}(r)$ and charge-one sector (odd number of fermions) $E_1^{(F)}(r)$. Neglecting $\frac{1}{2}$ compared with N in (10) we obtain

$$\mathscr{E}_0^{(F)}(r)=\lim_{N\to\infty}\frac{N}{\pi}(E_0^{(F)}(r)-E^{(F)})=r\qquad(r=2,3\ldots)\tag{11}$$

$$\mathscr{E}_1^{(F)}(r)=\lim_{N\to\infty}\frac{N}{\pi}(E_1^{(F)}(r)-E^{(F)})=\tfrac{1}{2}+r\qquad(r=1,2,\ldots).\tag{12}$$

The Virasoro algebra for the Ising model has central charge $c=\frac{1}{2}$ and the possible values of the lowest weights Δ of the irreducible representations are $\Delta=0$, $\frac{1}{2}$ and $\frac{1}{16}$ (Belavin *et al* 1984). For each representation Δ one can compute the degeneracy $d(\Delta,r)$ and this was done for us by Altschüler and Lacki (1985) using the character formula of Rocha-Caridi (1985). In table 1 we show the values of $d(\Delta,r)$ up to $r=10$. It is now a simple exercise to check, using (10) and table 1, that the spectrum $\mathscr{E}_0^{(F)}(r)$ is given by $\Delta=0$ (starting with the second descendent) and the spectrum $\mathscr{E}_1^{(F)}(r)$ is given by $\Delta=\frac{1}{2}$ (x_s is indeed $\frac{1}{2}$ for the spin-spin correlation (Cardy 1984)).

We now consider the three-state Potts quantum chain given by the Hamiltonian

$$H^{(F)}=-\frac{2}{3\sqrt{3}}\sum_{i=1}^{N}[\sigma_i+\sigma_i^++\lambda(\Gamma_i\Gamma_{i+1}^++\Gamma_i^+\Gamma_{i+1})]\qquad(\Gamma_{N+1}=0)\tag{13}$$

where

$$\sigma=\begin{pmatrix}1&0&0\\0&\omega&0\\0&0&\omega^2\end{pmatrix}\qquad\Gamma=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}\qquad\omega=\exp(\tfrac{2}{3}\pi\mathrm{i}).\tag{14}$$

The system has a critical point again at $\lambda=1$. The normalisation factor in (13) fixes the Euclidean time scale and it was found from our study of the model with periodic and twisted boundary conditions (von Gehlen *et al* 1986, von Gehlen and Rittenberg 1986b). The model is invariant under Z_3 (internal symmetry) and parity transformations and the Hamiltonian splits into six sectors with the corresponding spectra

$$E_Q^{(F)}(P,r)\qquad(Q=0,1,2;\ P=\pm)\tag{15}$$

Table 2. The spectrum $\mathscr{E}_0^{(F)}$ for the three-state Potts model in the charge-zero sector. The Van den Broeck–Schwartz approximants for the levels with positive parity ($\mathscr{E}_0^{(F)}(+)$) and negative parity ($\mathscr{E}_0^{(F)}(-)$) are given. The figure in brackets in the last two columns indicates the estimated error. On the left-hand side of the table we indicate the number of states having $\mathscr{E}_0^{(F)}=\Delta+r$ generated by the irreducible representations $\Delta=0$ and 3.

$\Delta+r$	(0)	(3)	$\mathscr{E}_0^{(F)}(+)$	$\mathscr{E}_0^{(F)}(-)$
2	1	—	2.000 (5)	—
3	1	1	—	2.99 (2), 2.98 (3)
4	2	1	4.004 (6), 3.995 (8), 4.01 (3)	—
5	2	2	—	4.98 (3), 4.98 (2), 5.00 (3), 4.99 (3)
6	4	3	5.97 (5), 5.98 (4), 5.99 (6), 5.8 (2)	—
7	4	4		7.0 (2), 6.9 (3), >6.6 (?)

where Q indicates the charge sector and P the parity. The symmetry under charge conjugation of the Hamiltonian gives the identity

$$E_1^{(F)}(P,r)=E_2^{(F)}(P,r) \tag{16}$$

and we are thus left to compute four spectra. According to (8) we have to determine the quantities

$$\mathscr{E}_Q^{(F)}(P,r)=\lim_{N\to\infty}\frac{N}{\pi}(E_Q^{(F)}(P,r)-E^{(F)}). \tag{17}$$

We have computed the energy levels $E_Q^{(F)}(P,r)$ for chains up to twelve sites using the Lanczos (1950) method. For up to seven sites we have checked the results by standard Householder diagonalisation (unlike in the periodic boundary case (von Gehlen and Rittenberg 1986b) here for up to seven sites there is no degeneracy of levels for finite chains). We then have calculated the Van den Broeck–Schwartz (1979) approximants for the $\mathscr{E}_Q^{(F)}(P,r)$. The results are shown in tables 2 and 3. Obviously we have been able to determine only the lower part of the spectrum but it turns out that we have determined enough levels for our purpose. Already the levels for finite chains cluster into several groups, which results in the approximate degeneracy of

Table 3. The spectrum $\mathscr{E}_1^{(F)}$ for the three-state Potts model in the charge-one sector. The Van den Broeck–Schwartz approximants for the levels with positive parity ($\mathscr{E}_1^{(F)}(+)$) and negative parity ($\mathscr{E}_1^{(F)}(-)$) are given. On the left-hand side of the table we indicate the number of states having $\mathscr{E}_1^{(F)}=\frac{2}{3}+r$ generated by the irreducible representation $\Delta=\frac{2}{3}$.

$\Delta+r$	$(\frac{2}{3})$	$\mathscr{E}_1^{(F)}(+)$	$\mathscr{E}_1^{(F)}(-)$
$\frac{2}{3}\simeq 0.6666\ldots$	1	0.6662 (4)	—
1.6666 ...	1	—	1.668 (2)
2.6666 ...	2	2.66 (1), 2.68 (4)	—
3.6666 ...	2	—	3.64 (4), 3.66 (2)
4.6666 ...	4	4.65 (4), 4.66 (3), 4.68 (3), 4.67 (2)	
5.6666 ...	5	—	5.58 (8), 5.65 (7), 5.65 (5), 5.66 (6), 5.66 (4)
6.6666 ...	8	6.6 (2), 6.55 (10)	—
7.6666 ...	10		>7.5 (?)

many levels $\mathscr{E}_Q^{(F)}(P, r)$ in tables 2 and 3. We are certainly missing higher levels, e.g. at $\mathscr{E}_0^{(F)}(+) \geq 6$, but we find exactly three levels around $\mathscr{E}_0^{(F)}(+) \simeq 4$.

In order to explain the spectra we recall that for the three-state Potts model the central charge of the Virasoro algebra is $c = \frac{4}{5}$ (Friedan *et al* 1984, Dotsenko 1984). The possible values of Δ in this case are

$$\Delta = 0, \tfrac{1}{40}, \tfrac{1}{15}, \tfrac{1}{8}, \tfrac{2}{5}, \tfrac{21}{40}, \tfrac{2}{3}, \tfrac{7}{5}, \tfrac{13}{8}, 3 \tag{18}$$

and the degeneracies $d(\Delta, r)$ are known (von Gehlen and Rittenberg 1986b). Comparing the 'experimental' spectra with the possible spectra generated by the irreducible representations given in (18) we notice that the spectrum

$$\mathscr{E}_0^{(F)} = \mathscr{E}_0^{(F)}(+) + \mathscr{E}_0^{(F)}(-) \tag{19}$$

is obtained considering the representations with $\Delta = 0$ and 3. This can be seen comparing the left-hand side of table 2, where the number of states corresponding to each level is given, and the right-hand side of table 2, where the 'experimental' data are shown. It is interesting to notice that from our short chains we have been able to identify the whole spectrum (any Δ from (18) would have shown up since we have found the largest one $\Delta = 3$). A similar analysis for the charge-one sector

$$\mathscr{E}_1^{(F)} = \mathscr{E}_1^{(F)}(+) + \mathscr{E}_1^{(F)}(-) \tag{20}$$

shows that the spectrum is given by the irreducible representation $\Delta = \frac{2}{3}$.

To summarise, we have identified the irreducible representations which give the finite-size limit of the spectra of the Ising and three-state Potts Hamiltonians with free boundary conditions. They are

$$\begin{array}{lll} \mathscr{E}_0^{(F)} = (0) & \mathscr{E}_1^{(F)} = (\frac{1}{2}) & \text{(Ising)} \\ \mathscr{E}_0^{(F)} = (0), (3) & \mathscr{E}_1^{(F)} = \mathscr{E}_2^{(F)} = (\frac{2}{3}) & \text{(three-state Potts).} \end{array} \tag{21}$$

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