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Conformal invariance and surface critical behaviour of a quantum chain with three-spin interaction

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Abstract. An Ising model with three-spin interaction is investigated by finite-size scaling applying free boundary conditions. The surface critical properties of the model were determined by conformal invariance. Taking into account logarithmic corrections the surface critical exponents obtained are in accordance with the four-state Potts values.

Recently models with many-body interactions have received increasing attention. It is now known from some exact results (Baxter 1972, Baxter and Wu 1973) that the critical properties of these models generally depend on the range of the interaction. Recently considerable effort has been made to clarify the critical properties of the following simple one-dimensional quantum model described by the Hamiltonian (Turban 1982, Penson *et al* 1982):

$$H = -\lambda \sum_i \sigma_i^x \sigma_{i+1}^x \ldots \sigma_{i+m-1}^x - h \sum_i \sigma_i^z \qquad (1)$$

where σ_i^x and σ_i^z denote the Pauli matrices at site i. The classical statistical mechanical equivalent of this model is a two-dimensional square lattice Ising model with mixed m-spin and two-spin interactions.

The Hamiltonian (1) is self-dual (Turban 1982, Penson *et al* 1982), the self-dual point being $h = \lambda$ independent of m. There is one phase transition in the system, which turns from second order to first order, when $m > m_c$. By now it is established that $m_c = 3$ (Iglói *et al* 1986, Blöte *et al* 1986b, Alcaraz 1986). However, the situation with the universality class of the $m = 3$ model was controversial. The first numerical results (Penson *et al* 1982, Iglói *et al* 1983, 1986, Debierre and Turban 1983, Kolb and Penson 1986) were significantly different from those of the four-state Potts model, not supporting the conjecture of Debierre and Turban (1983) that the two models belong to the same universality class. More recently, however, a mapping has been revealed between the two models (Blöte 1987) which becomes exact in the very anisotropic limit. Recent numerical results on the bulk critical properties—taking into account the effect of logarithmic corrections—confirm the validity of the above mapping (Blöte *et al* 1986b, Alcaraz and Barber 1987, Vanderzande and Iglói 1987). Furthermore the critical properties of the model (1) seem to be independent of the value of the spin for $m = 2$ and $m = 3$ (Iglói *et al* 1987).

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In this paper we extend the investigations to the surface critical behaviour of the $m=3$ model. Our aim in the present work is twofold: (i) to justify the equivalence in the surface critical behaviour between the $m=3$ model and the four-state Potts model, and (ii) to obtain more accurate numerical results on the surface critical exponents of models in the four-state Potts universality class.

The surface critical exponents of the q-state Potts model have been conjectured by Cardy (1984) using conformal invariance. According to his results the anomalous dimension of the surface spin-spin correlations $x'_s = \eta_\parallel/2$ is

$$x'_s = (m-1)/(m+1) \tag{2}$$

where

$$\sqrt{q} = 2\cos[\pi/(m+1)] \tag{3}$$

and m is an odd integer. Thus $q=4$ corresponds to $m=\infty$, and then $x'_s=1$. On the other hand the anomalous dimension of the surface energy-energy correlations x'_ε is independent of the value of q (Diehl *et al* 1983, Cardy 1984): $x'_\varepsilon = 2$.

The validity of the above conjectures has been investigated in several papers. For $q=2$ x'_s coincides with the exact result on the Ising model (Pfeuty 1970, Burkhardt and Guim 1985) and for $q=3$ numerical calculations (Droz *et al* 1985, von Gehlen and Rittenberg 1986) support the validity of (2). However, for $q=4$ the first numerical results were significantly different from $x'_s=1$. Droz *et al* (1985) obtained $x'_s=0.77$, and von Gehlen *et al* (1986) $x'_s=0.905$. The reason for these discrepancies, as was pointed out by Vanderzande and Stella (1987), is the effect of logarithmic corrections (Nauenberg and Scalapino 1980, Cardy *et al* 1980). By taking these corrections properly into account Vanderzande and Stella (1987) were able to verify numerically Cardy's (1984) conjecture.

In this paper the ground-state properties of the $m=3$ model in (1) are determined for finite chains using free boundary conditions. Then the surface critical properties are obtained from these data using conformal invariance (Cardy 1987). The method of conformal invariance has already been applied for the $m=3$ model by Kolb and Penson (1986) and Alcaraz and Barber (1987) to determine the bulk critical properties. In this case periodic boundary conditions have to be applied, which restrict the possible length of the finite chains as $L=3*l$ $(l=1,2,\ldots)$. For free chains there is no such restriction (Iglói *et al* 1983), thus much more finite-size data are available.

In the following we briefly describe the symmetry properties of the low lying energy levels of free chains (Iglói *et al* 1983). The spectrum of the Hamiltonian splits into four disjoint sectors. The zeroth sector is non-degenerate. It is characterised by the state $++++\ldots+$, and for finite chains it contains the ground state of the system. The first, second and third sectors are characterised by the states: $-+++\ldots+$, $+-++\ldots+$ and $++-+\ldots+$, respectively. These three sectors are degenerate for infinite chains (and also for periodic finite chains), but for free finite chains there are always two degenerate and one non-degenerate sectors. For $L(\text{mod } 3)=0,1,2$, the second, the first and the third sectors are non-degenerate, respectively. In the following the kth energy level in the nth sector is denoted by $E_{n,k}$ $(n=0,1,2,3;\ k=0,1,\ldots)$.

According to conformal invariance (Cardy 1987, von Gehlen and Rittenberg 1986) these energy levels satisfy the following relations at the bulk critical point $h=\lambda$:

$$\lim_{L\to\infty}(L/\pi)(E_{n,k}-E_{0,0}) = (x_n+k')\xi\begin{cases} n=0,\ k'=k-1=0,1,\ldots \\ n\neq 0,\ k'=k=0,1,\ldots. \end{cases} \tag{4}$$

Here $x_0 = x'_\varepsilon$ and $x_1 = x_2 = x_3 = x'_s$ are the anomalous dimensions of the energy and the spin operators at the surface, respectively. ξ is the sound velocity appearing in the Hamiltonian formalism, since a Hamiltonian may be multiplied in principle with any constant.

In addition the central charge c of the Virasoro algebra may be determined from the finite-size corrections to the ground-state energy at $\lambda = h$ (Blöte *et al* 1986a, Affleck 1986):

$$E_{0,0}/L = a_0 + a_1/L - \pi c\xi/24L^2 + \sigma(1/L^2). \qquad (5)$$

In practice we calculate the energy levels $E_{n,k}$ for $n = 0, 1, 2, 3$ and $k = 0, 1$ for free chains up to $L = 17$. The numerical solution of the eigenvalue problem was performed by the Lánczos method as described by Patkós and Ruján (1985). We have found that the energy levels for $n = 1$, 2 and 3 determine the same anomalous dimension x_n. However, the boundary conditions influence the various gaps differently. In order to decrease the systematic fluctuations present in the individual gaps, we averaged over the energy levels for $n = 1$, 2 and 3, as previously done in the paper of Iglói *et al* (1983). In the following we use the notation

$$\bar{E}_{1,k} = \tfrac{1}{3}(E_{1,k} + E_{2,k} + E_{3,k}) \qquad (6)$$

for the averaged energy levels.

The various scaled gaps for different lengths of the chain are presented in table 1 together with the extrapolated values. The errors in the extrapolation are due to two facts. The series contain systematic deviations by modulo 3 and the different series show strong corrections to scaling. From the numerical data one obtains $1/(\log L)$ corrections to the first series and $1/L$ corrections to the last two series. From the ratio of the extrapolated values given in table 1, one can estimate $x'_s = 1.0 \pm 0.06$ and $x'_\varepsilon = 2.0 \pm 0.1$ in accordance with the four-state Potts values as conjectured by Cardy (1984). The extrapolated value of the sound velocity $\xi = 3.15 \pm 0.1$ is in accordance with the findings of Alcaraz and Baxter (1987) and coincides (within errors) with the

Table 1. The various scaled gaps for different lattice sizes. Extrapolated values are presented at the foot of each column.

L	$(\bar{E}_{1,0} - E_{0,0})L/\pi$	$(E_{0,1} - E_{0,0})L/\pi$	$(\bar{E}_{1,1} - \bar{E}_{1,0})L/\pi$
3	1.669 28	4.370 23	2.700 95
4	1.867 96	4.733 85	2.809 29
5	1.987 52	5.000 92	2.212 65
6	2.069 24	5.288 53	2.021 73
7	2.134 83	5.453 61	2.254 25
8	2.184 52	5.584 09	2.421 62
9	2.224 73	5.688 54	2.527 93
10	2.259 09	5.762 31	2.616 85
11	2.287 78	5.824 73	2.683 08
12	2.312 55	5.876 31	2.732 50
13	2.334 50	5.916 84	2.776 20
14	2.353 74	5.952 23	2.810 57
15	2.370 94	5.982 56	2.838 51
16	2.386 53	6.007 88	2.863 76
17	2.400 61	6.030 47	2.884 56
Ext	$\xi x'_s = 3.2 \pm 0.1$	$\xi x'_\varepsilon = 6.35 \pm 0.1$	$\xi = 3.15 \pm 0.1$

value of the Hamiltonian four-state Potts model: $\xi = 3.16$ (von Gehlen *et al* 1986). It means that not only the critical exponents are the same in the two models but the sound velocities as well.

In the following we shall try to decrease the extrapolation errors, by taking into account logarithmic corrections in the same form as in the four-state Potts model. The appearance of logarithmic singularities in the four-state Potts model is the consequence of a marginal scaling field, denoted by ψ, which appears besides the other scaling fields. In our case these are the energy (temperature) in the bulk (φ) and on the surface (φ'), and the magnetic field in the bulk (h) and on the surface (h'). Following the work of Nauenberg and Scalapino (1980), Cardy *et al* (1980) and Blöte and Nightingale (1982), Vanderzande and Stella (1987) have recently shown that the scaling form of the free energy of the four-state Potts model is

$$f(\varphi, \varphi', h, h', \psi, L) = L^{-2} f(L^{2-x_\varepsilon} z^{3/4}\varphi, L^{1-x'_\varepsilon}\varphi', L^{2-x_s} z^{1/16} h, L^{1-x'_s} z^{-1} h', z\psi, 1) \tag{7}$$

where

$$z = [1 - (\psi(0)/\pi) \log L]^{-1} \tag{8}$$

and L is the linear size of the system. From these equations it is easy to read the strength of the leading logarithmic corrections. x'_ε has no such corrections (it is a consequence of the fact that x'_ε does not depend on q), while the leading finite-size correction to x'_s

$$x'_s(L) = x'_s - 1/\log L + b/(\log L)^2 \tag{9}$$

is universal in accordance with Cardy (1986). Here $x'_s(L)$ denotes the effective exponent obtained by a two-point fit. Now following the strategy of Blöte *et al* (1986b) and Vanderzande and Iglói (1987), we plot in figure 1 the expression $x'_s(L) + 1/\log L$ with respect to $1/(\log L)^2$. As is seen the effective exponents for different L lie close to a straight line, and with relatively small errors, an extrapolation can be performed yielding $x'_s = 1.00 \pm 0.02$. Now repeating the analysis for the x'_ε exponent, by taking

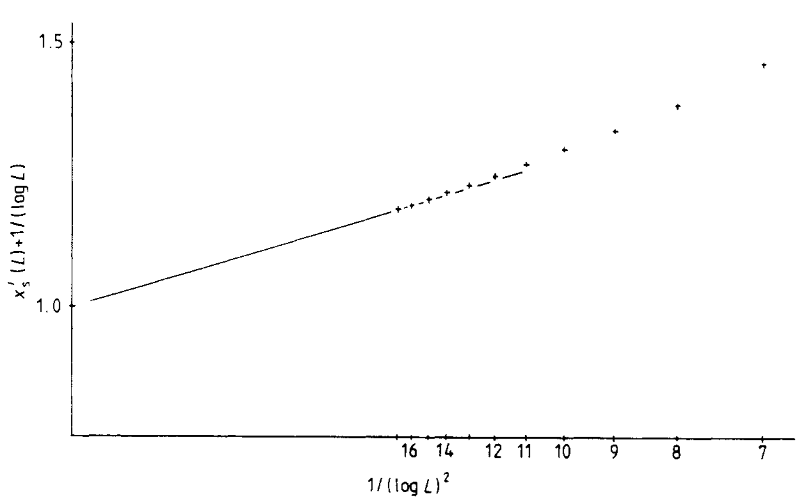

Figure 1. The effective exponent $x_s(L) + 1/\log L$ as a function of $1/(\log L)^2$.

the ratio of the values present in the last two columns of table 1, one obtains $x'_\varepsilon = 2.00 \pm 0.03$ in very good agreement with the theoretical predictions (Cardy 1984).

Finally we turn to the question of the determination of the central charge of the Virasoro algebra, by using the relation (5). Since neither the ground-state energy, nor the surface energy term is known exactly for the infinite system, a_0, a_1 and $c\xi$ can thus be obtained by a three-point fit. The results evaluated from the finite lattice data with lattice sizes L, $L-3$ and $L-6$ are presented in table 2. As is seen the effect of confluent singularities on $c\xi$ is extremely strong. For periodic chains according to Cardy (1986) the effective $c(L)$ values should approach their limit from above as $1/(\log L)^3$. For free chains, the general theory is not available, but for the quantum XXZ chain Woynarovich (1987) has shown that the first logarithmic correction is $c(L) = c + \alpha/(\log L)^2$, where $\alpha < 0$. In our case the calculated $c(L)$ values also obey this relation, and the extrapolated value of the central charge $c = 0.95 \pm 0.07$ is in accordance with the $c = 1$ characteristic for models in the four-state Potts universality class (Cardy 1987).

Table 2. Three-point fit estimates for the central charge from equation (5). The finite lattice results for L, $L-3$ and $L-6$ were compared.

L	a_0	a_1	$c\xi$
9	−1.197 58	0.5105	1.835
10	−1.197 81	0.5137	1.913
11	−1.197 94	0.5158	1.971
12	−1.198 05	0.5176	2.029
13	−1.198 12	0.5190	2.083
14	−1.198 17	0.5201	2.125
15	−1.198 21	0.5210	2.164
16	−1.198 24	0.5217	2.199
17	−1.198 26	0.5223	2.230

To summarise we have determined the surface critical properties of a three-spin coupling model by conformal invariance. The obtained anomalous dimensions $x'_s = 1.00 \pm 0.02$ and $x'_\varepsilon = 2.00 \pm 0.03$ are in very good agreement with Cardy's (1984) conjecture for the four-state Potts model. Comparing our calculation with those performed with periodic boundary conditions, we can say that in our case about three times more finite lattice points are available. A similar comparison with the four-state Potts model (von Gehlen *et al* 1986) shows about twice as many finite lattice results in our calculation. Thus we can conclude that our results supply the most accurate numerical evidence to verify the following two conjectures: (i) the $m = 3$ model and the four-state Potts model belong to the same universality class and (ii) the surface magnetic exponent of the four-state Potts model is given by (2).

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