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LETTER TO THE EDITOR

Bulk and surface critical behaviour at the conformal invariant point in the Z_5 model

C Vanderzande

Limburgs Universitair Centrum, Departement WNIF, Universitaire Campus, B-3610 Diepenbeek, Belgium

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Abstract. We determine the bulk thermal and magnetic exponents at the conformal invariant point in the Z_5 model with a Monte Carlo based finite-size calculation. Our results are in good agreement with the predictions of Zamolodchikov and Fateev. We also argue that the $(N-1)$ surface magnetic exponents $x_h(j)$ in the Z_N model are given by $j(N-j)/N$ ($j=1, \dots, N-1$). This prediction is also verified in a Monte Carlo finite-size calculation for the Z_5 model.

The idea that at critical points systems are not only scale invariant but invariant under all conformal transformations has led to many interesting developments, especially for two-dimensional systems (for a review, see Cardy (1986) or Itzykson (1986)).

So far the main interest has been focused on theories where the central charge c of the Virasoro algebra is less than or equal to one. In these cases, unitarity severely limits the possible values of the critical exponents (Friedan *et al* 1984). These theories describe such well known models as the Ising, Potts or $O(N)$ model.

More recently, Zamolodchikov and Fateev (1985, hereafter referred to as ZF) constructed a conformal quantum field theory which is self-dual and has Z_N symmetry. For these theories, the central charge is found to be

$$c = 2(N-1)/(N+2) \quad (1)$$

meaning that $c > 1$ for $N \geq 5$. Furthermore, ZF predict all possible anomalous dimensions x of operators in the theory. They find that the leading thermal exponent is given by

$$x_t = 4/(N+2) \quad (2a)$$

whereas the dimensions of the $(N-1)$ order parameters which are present in the theory are given by

$$x_h(j) = j(N-j)/N(N+2) \quad j = 1, \dots, N-1. \quad (2b)$$

(These exponents x are related to the more familiar exponents y , by $x+y=d=2$). These exponents precisely correspond to exponents which were found by Huse (1984) in a restricted SOS model (Andrews *et al* 1984). However, ZF suggest that the exponents (2) should also be the exponents of the critical points which are present in Z_N models (Fateev and Zamolodchikov 1982).

In the present letter we want to verify this conjecture in the case of the Z_5 model. This is the simplest of the Z_N models which cannot be reduced to Ising or Potts models. Furthermore we will not only study the bulk critical exponents given by (2), but also the surface exponents which were so far unknown.

A study of the Z_5 model similar to the present one has been performed by Alcaraz (1986), who works on a one-dimensional quantum version of the Z_5 model. However, he only considered bulk critical behaviour.

In the Z_5 model one has at each site a variable n_i which can take on the values $1, 2, \dots, 5$. The most general (reduced) Hamiltonian involving only nearest-neighbour interactions consistent with Z_5 symmetry is then given by:

$$H = K_1 \sum_{\langle i,j \rangle} \cos \frac{2\pi}{5} (n_i - n_j) + K_2 \sum_{\langle i,j \rangle} \cos \frac{4\pi}{5} (n_i - n_j). \quad (3)$$

The phase diagram of this model has been intensively studied in the past (Cardy 1980, Alcaraz and Köberle 1980, Fateev and Zamolodchikov 1982), and is found to have a rich structure including first-order transitions, massless phases and two second-order transitions. One of these occurs at $K_1^* = 0.577$ and $K_2^* = 0.368$ (Fateev and Zamolodchikov 1982), the other one is related to this first one by a simple symmetry and thus has the same exponents. If this critical point is described by the conformal theory of Z_F , we have from (2a) that the thermal exponent at this point should be $y_t = 10/7$.

The model has four order parameters which are related, two by two, by Z_N symmetry. The two independent order parameters can be chosen as:

$$M_1 = \langle \delta_{n_i,1} - \delta_{n_i,2} \rangle \quad (4a)$$

and

$$M_2 = \langle \delta_{n_i,1} - \delta_{n_i,3} \rangle. \quad (4b)$$

In the neighbourhood of the point K_1^*, K_2^* it is energetically more favourable to have $n_i - n_j = \pm 1$ than to have $n_i - n_j = \pm 2$. As a consequence we will have $M_1 \leq M_2$. Because both order parameters have to vanish at the critical point, it follows that the magnetic exponent of M_2 should be larger than the exponent of M_1 . Using (2b) we thus find the magnetic exponents $y_h(2) = 64/35$ and $y_h(1) = 66/35$ for M_1 and M_2 respectively.

We now want to verify these predictions using the technique of finite-size scaling (Barber 1983). For the Z_5 model the specific heat in a finite system of size L , at the infinite systems critical point K_1^*, K_2^* , is expected to behave as

$$C_L(K_1^*, K_2^*) \sim L^{-d+2y_t} \sim L^{6/7}. \quad (5a)$$

The two independent susceptibilities (corresponding to fluctuations in the respective order parameters M_1 and M_2) should behave as:

$$\chi_L^{(1)}(K_1^*, K_2^*) \sim L^{-d+2y_h(2)} \sim L^{58/35} \quad (5b)$$

and

$$\chi_L^{(2)}(K_1^*, K_2^*) \sim L^{-d+2y_h(1)} \sim L^{62/35}. \quad (5c)$$

We have calculated $C_L(K_1^*, K_2^*)$, $\chi_L^{(1)}(K_1^*, K_2^*)$ and $\chi_L^{(2)}(K_1^*, K_2^*)$ with the Monte Carlo method for square systems with side $L = 2, 4, \dots, 18$, using periodic boundary conditions. For the largest system sizes it was necessary to do up to $1.5-2 \times 10^6$ MCS/spin in order to obtain sufficient convergence.

Errors were obtained from fluctuations in subresults. For each system size at least two independent runs were performed. As an example of our results, we show in figure 1 our data for $C_L(K_1^*, K_2^*)$ and $\chi_L^{(2)}(K_1^*, K_2^*)$.

We analysed our results in two ways. First, we determined the exponents from a simple log-log plot. This gave (between brackets we give the conjectured result)

$$\begin{aligned} y_t &= 1.44 \pm 0.02 && (1.429) \\ y_h(1) &= 1.89 \pm 0.02 && (1.886) \\ y_h(2) &= 1.83 \pm 0.02 && (1.829). \end{aligned} \quad (6)$$

Secondly, the finite-size data were considered as coefficients of a series which can then be analysed by a dlog Padé method. For example, in the case of the specific heat, the series

$$\sum_L C_L(K_1^*, K_2^*) z^L \quad (7)$$

is expected to behave as $(z-1)^{d-2y_t-1}$ near $z=1$. This method to extract exponents has already been applied to some problems in random fractals (Stella *et al* 1986) and to the surface critical behaviour of the q -state Potts model (Vanderzande and Stella 1987). The method gives accurate estimates of exponents, because it takes into account the 'global' behaviour of data, so that 'local' fluctuations (which are of course present in MC data) are washed out to some extent. (More usual extrapolation methods such as the Van den Broeck-Schwarz (1979) method fail for data with noise.) From this analysis we find:

$$y_t = 1.44 \pm 0.02 \quad y_h(1) = 1.88 \pm 0.03 \quad y_h(2) = 1.84 \pm 0.03. \quad (8)$$

We thus see that our data, (6) and (8), beautifully confirm the conformal predictions. Most of all, this justifies the identification, made by Z_P , of the critical points in the Z_N model with their Z_N conformal quantum field theory. We also mention that this conclusion is in agreement with the work of Alcaraz (1986).

We now turn to the surface critical behaviour, which occurs if we study a semi-infinite system (Binder 1983). Here we are interested in the ordinary transition, i.e. in the case where surface and bulk couplings are equal. The surface critical exponents

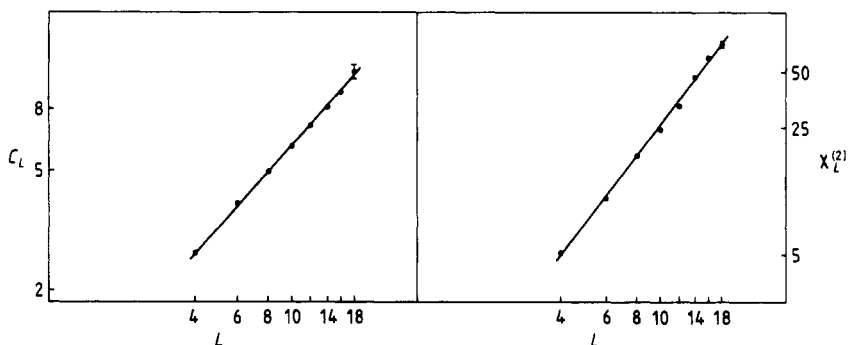


Figure 1. The specific heat C_L and the susceptibility $\chi_L^{(2)}$ at the Z_5 critical point as a function of system size L . The dots are our Monte Carlo data, the full lines give best fits through these data. The estimated error in the data is indicated for $L=18$. For smaller systems the error is correspondingly smaller.

of the Z_N model were not identified by Z_P , nor were they studied in the work of Alcaraz (1986). From Burkhardt and Cardy (1986) we know that the surface thermal exponent x'_t in this case equals two. We therefore turn to the surface magnetic exponents and first find which exponents out of the complete set predicted by Z_P correspond to surface exponents in the case of the Z_2 (Ising) and Z_3 ($q=3$ Potts) models. For these models the surface exponents are known from conformal invariance for models with $c < 1$ (Cardy 1984). We then assume, as Cardy (1984) did for the Potts and $O(N)$ models, that these same exponents describe the surface behaviour for all N . In this way we find for the $(N-1)$ surface exponents $x'_h(j)$

$$x'_h(j) = j(N-j)/N \quad (j = 1, \dots, N-1). \quad (9)$$

(The more familiar exponents $y'_h(j)$ are given by $1 - x'_h(j)$.) We also verified this prediction in the case of the Z_5 model. As we already did for the surface behaviour of the Potts model (Vanderzande and Stella 1987), we calculate $x'_h(j)$ by calculating the surface susceptibility. For the Z_5 model, there are two such quantities given by

$$\chi_L^{(1)}(K_1^*, K_2^*) = \frac{1}{L^d} \sum_{\substack{i \in S \\ j \in V}} [\langle (\delta_{n,1} - \delta_{n,2})(\delta_{n,1} - \delta_{n,2}) \rangle - \langle (\delta_{n,1} - \delta_{n,2}) \rangle \langle (\delta_{n,1} - \delta_{n,2}) \rangle] \quad (10)$$

where V indicates the whole volume (including the surface S). A similar equation (with state 2 replaced by state 3) holds for $\chi_L^{(2)}(K_1^*, K_2^*)$. According to finite-size scaling and equations (2) and (9) they should behave as:

$$\chi_L^{(1)}(K_1^*, K_2^*) \sim L^{-d+y_h(2)+y'_h(2)} \sim L^{-13/35} \quad (11a)$$

and

$$\chi_L^{(2)}(K_1^*, K_2^*) \sim L^{-d+y_h(1)+y'_h(1)} \sim L^{3/35}. \quad (11b)$$

The surface susceptibilities were calculated with the Monte Carlo using periodic boundaries conditions in one direction, and free boundaries in the other, thus creating a surface S . The calculations were performed for the same system sizes as for the bulk properties. Once more, the results were analysed by a simple straight line fit to the log-log of the data which gave

$$-d + y_h(1) + y'_h(1) = 0.08 \pm 0.03 \quad (0.086) \quad (12a)$$

and a dlog Padé analysis which gives

$$-d + y_h(1) + y'_h(1) = 0.08 \pm 0.03. \quad (12b)$$

In the case of $\chi_L^{(1)}$, one must be more careful. Indeed, beside the singular term which is given by (11a), there is also a regular contribution to $\chi_L^{(1)}$, which was shown to be proportional to $1/L$ (Vanderzande and Stella 1987). Such a term is always present but can be neglected unless one considers quantities whose singular contribution goes to zero. Therefore we looked at the quantity $\chi_L^{(1)}(K_1^*, K_2^*) \cdot L$ which should behave as:

$$\chi_L^{(1)}(K_1^*, K_2^*) \cdot L \approx a_0 + a_1 \cdot L^z \quad (13)$$

where a_0 and a_1 are constants and z should be equal to $22/35 = 0.629$. We fitted our MC data to this form. The best fit (meaning chi-squared minimal) was found for $z = 0.67$ (see figure 2). However we must note that in the whole region $0.62 < z < 0.67$, the chi-squared value was nearly constant.

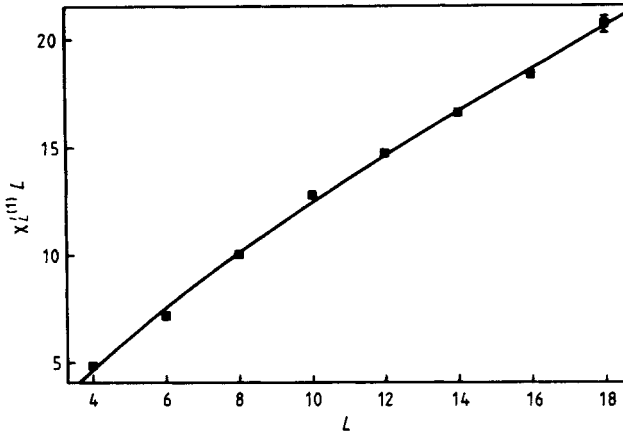


Figure 2. The surface susceptibility $\chi_L^{(1)}L$ as a function of system size L . The dots indicate our data, the full curve $(-4.49 + 3.64L^{0.67})$ is the best fit through the data. An estimate of the error is indicated for $L = 18$.

We may thus conclude that the prediction (9) is, at least in the case of the Z_5 model, verified by our Monte Carlo calculations. Thus, it is also fair to say that now both bulk and surface exponents of the Z_N model are probably known exactly, just as was already the case for the Potts and $O(N)$ models.

We would like to make one final remark. Equations (2) and (7) imply the scaling relation

$$x'_h(j) = 4x_h(j)/x_l. \quad (14)$$

It is remarkable that this scaling relation also holds for the Potts model and the tricritical Potts model (Vanderzande and Stella 1987). Using the results from Cardy (1984) it is furthermore seen to hold in the $O(N)$ model ($-2 \leq N \leq 2$). However it is not valid in, e.g., the 3D Ising model. Therefore, (14) might possibly be a general consequence of 2D conformal invariance. So far however, we have not been able to prove this idea.

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