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1994 J. Phys. A: Math. Gen. 27 L223

(http://iopscience.iop.org/0305-4470/27/8/001)

J. Phys. A: Math. Gen. 27 (1994) L223–L230. Printed in the UK

LETTER TO THE EDITOR

CFT estimates of the universal Binder parameter for quantum ground-state transitions in one dimension

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Received 4 January 1994

Abstract. The universal values of the equal-time Binder parameter for quantum ground-state transitions in one dimension are predicted with the help of the conformal field theory (CFT) in two dimensions. The values are compared with the results from the numerical diagonalization of the $S = 1$ antiferromagnetic XXZ chain. It is found that the finite-size corrections may be of a higher order in L^{-1} than expected.

Understanding of phase transitions in two dimensions has been greatly developed since an infinite number of conformal symmetries of the two-dimensional massless theory were discovered [1, 2]; see [3] for a review. The application of the theory particularly to finite-size scaling of one-dimensional quantum systems [4, 5] is of practical importance from the viewpoint of numerical studies. Comparison between numerical data for finite systems and predictions of the conformal field theory can reveal the central charge c, or the universality class of a transition.

It seems that numerical studies in this context have, so far, been rather restricted to calculations of the energy spectrum; there have been only a limited number of studies on physical quantities at the ground state [6, 7]. It is useful to predict the finite-size behaviour of physical quantities by means of the conformal field theory; in some cases, e.g. in calculations by quantum Monte Carlo methods [8], it is much easier to obtain physical quantities than to obtain the energy spectrum.

An especially important quantity is the Binder parameter [9, 10]:

$$U(\lambda; L) \equiv 1 - \frac{\left\langle 0 \middle| \left(\sum_{i=1}^{L} \mathcal{O}_i\right)^4 \middle| 0 \right\rangle}{3\left\langle 0 \middle| \left(\sum_{i=1}^{L} \mathcal{O}_i\right)^2 \middle| 0 \right\rangle^2} \tag{1}$$

where λ is a parameter embedded in the Hamiltonian of a system of size L, the state $|0\rangle$ denotes the ground state, and $\mathcal{O}_i$ is the relevant order-parameter operator at the site i. The Binder parameter is one of the critical-amplitude ratios (see [11] for a review), and is expected to be dimensionless and universal at the critical point

$$U(\lambda_c; L) = U^* = \text{constant}. \tag{2}$$

In the present letter we numerically estimate the universal constant (2) for the critical theories with $c = \frac{1}{2}$ and $c = 1$, and compare the estimates with the results of a numerical-diagonalization study of the $S = 1$ antiferromagnetic XXZ chain.

0305-4470/94/080223+08\$19.50

In a previous study [12], another version of the Binder parameter, which is based on the response functions, was found to be universal:

$$U_{\text{response}} \equiv 1 - \frac{\chi^{(4)}}{3\left(\chi^{(2)}\right)^2} = 1 + \frac{2}{\pi\eta} \qquad \text{for} \quad \lambda = \lambda_c \tag{3}$$

in the limit of small η, where η is the correlation exponent, and $\chi^{(2)}$ and $\chi^{(4)}$ denote the linear and the nonlinear response functions, respectively. From the viewpoint of numerical studies, however, it is easier to estimate (1) than to estimate (3); the quantities $\langle 0|(\sum \mathcal{O}_i)^n|0\rangle$ consist only of the equal-time correlations of the operators $\{\mathcal{O}_i\}$, while calculation of the response functions involves the matrix inversion, the numerical differentiation or the evaluation of all the different-time correlations. Hence we consider that it is an important and unsolved problem to predict the universal value of the equal-time Binder parameter (1) by means of the conformal field theory.

Let us describe how to compute the equal-time Binder parameter of the massless theory.

With the help of the conformal field theory in two dimensions, we can write down multi-point correlation functions on an infinite plain. On the other hand, we can describe a one-dimensional periodic quantum system of length L in terms of the field theory on a cylinder of circumference L. The axis u across the cylinder corresponds to the real-space direction, while the axis v along it corresponds to the inverse temperature, or the imaginary time direction.

We obtain the cylinder geometry from the infinite plain by means of the following conformal map [4]:

$$w = \frac{L}{2\pi} \ln z \tag{4}$$

where $z \equiv x + \mathrm{i}y$ is the complex coordinate of the plain, and $w \equiv u + \mathrm{i}v$ is that of the cylinder. The correlation functions on the cylinder relate to those on the plain in the form

$$\langle \mathcal{O}(z_1)\mathcal{O}(z_2)\ldots\mathcal{O}(z_N)\rangle_{\text{plain}} = \left(\frac{L}{2\pi}\right)^{N\eta/2} \prod_{j=1}^{N} |z_j|^{-\eta/2} \langle \mathcal{O}(w_1)\mathcal{O}(w_2)\ldots\rangle_{\text{cyl}} . \tag{5}$$

Here $\eta/2$ is the scaling dimension of the operator $\mathcal{O}$.

The equal-time correlations of the one-dimensional quantum system in the ground state are given by

$$\langle 0\,|\mathcal{O}(v_1)\mathcal{O}(v_2)\ldots|\,0\rangle = \langle \mathcal{O}(w_1)\mathcal{O}(w_2)\ldots\rangle_{\text{cyl}}\Big|_{u_1=u_2=\cdots=0} . \tag{6}$$

We thus obtain the moments of the order parameter in the forms

$$\left\langle 0\left|\left(\sum \mathcal{O}_i\right)^n\right|0\right\rangle \simeq \int\cdots\int_0^L \prod_{j=1}^{n} \mathrm{d}v_j \, \langle 0\,|\mathcal{O}(v_1)\mathcal{O}(v_2)\cdots|\,0\rangle . \tag{7}$$

These provide the explicit expression of (1) at the critical point.

In the following we derive formulae for the universal values of the equal-time Binder parameter (2) for $c = \frac{1}{2}$ and $c = 1$.

First we consider the critical theory with the central charge $c = \frac{1}{2}$, namely the theory of the two-dimensional Ising universality class. The scaling dimension of the order-parameter operator [1, 2] is $\frac{1}{2}\eta = \frac{1}{8}$. We write down the two-point correlation function on the infinite plain in the form

$$\langle \mathcal{O}(z_1)\mathcal{O}(z_2)\rangle_{\text{plain}} = \frac{A^2}{|z_{12}|^{1/4}} \tag{8}$$

where $z_{jk} \equiv z_j - z_k$, and A denotes an amplitude factor. The four-point correlation function is given by [2, 13–15]

$$\langle \mathcal{O}(z_1)\mathcal{O}(z_2)\mathcal{O}(z_3)\mathcal{O}(z_4)\rangle_{\mathrm{plain}} = \frac{A^4}{\sqrt{2}} \left| \frac{z_{12}z_{34}}{z_{13}z_{14}z_{23}z_{24}} \right|^{1/4} \sqrt{1 + |\zeta| + |1-\zeta|} . \tag{9}$$

Here the cross ratio ζ is defined as follows:

$$\zeta \equiv \frac{z_{13}z_{24}}{z_{12}z_{34}} . \tag{10}$$

The conformal map (4) gives the correlation functions on the cylinder in the forms

$$\langle \mathcal{O}(w_1)\mathcal{O}(w_2)\rangle_{\mathrm{cyl}} = \left(\frac{\pi}{L}\right)^{1/4} \frac{A^2}{|s_{12}|^{1/4}} \tag{11}$$

and

$$\langle \mathcal{O}(w_1)\mathcal{O}(w_2)\mathcal{O}(w_3)\mathcal{O}(w_4)\rangle_{\mathrm{cyl}} = \left(\frac{\pi}{L}\right)^{1/2} \frac{A^4}{\sqrt{2}} \left[\left| \frac{s_{12}s_{34}}{s_{13}s_{14}s_{23}s_{24}} \right|^{1/2} + (2 \leftrightarrow 3) + (2 \leftrightarrow 4) \right]^{1/2} \tag{12}$$

with

$$s_{jk} \equiv \frac{1}{2} \frac{z_{jk}}{\sqrt{z_j z_k}} = \sinh \frac{\pi}{L}(u_{jk} + \mathrm{i}v_{jk}) . \tag{13}$$

The second and the third terms in the right-hand side of (12) symmetrize the expression with respect to the subscripts. For example, the second term has the same form as the first term except that its subscripts '2' and '3' are exchanged. We put $u_{jk} = 0$ as in (6), and obtain the equal-time correlations in the forms (11) and (12) with s_{jk} reduced to

$$s_{jk} = \mathrm{i} \sin \frac{\pi}{L} v_{jk} . \tag{14}$$

The equal-time moments of the order parameter are given by (7).

We thus obtain the final formula of the critical-point Binder parameter (2) for the Ising universality class in the following form:

$$U_{\mathrm{I}}^* = 1 - \frac{1}{3\sqrt{2}\pi^2} \frac{b_{\mathrm{I}}}{a_{\mathrm{I}}^2} \qquad \text{for} \quad c = \tfrac{1}{2} \tag{15}$$

with

$$a_{\mathrm{I}} \equiv \frac{\Gamma(\frac{3}{8})}{\Gamma(\frac{7}{8})} \tag{16}$$

and

$$b_{\mathrm{I}} \equiv \int\!\!\int\!\!\int_0^{\pi} \mathrm{d}\theta_2\, \mathrm{d}\theta_3\, \mathrm{d}\theta_4 \left[\left| \frac{s_{12}s_{34}}{s_{13}s_{14}s_{23}s_{24}} \right|^{1/2} + (2 \leftrightarrow 3) + (2 \leftrightarrow 4) \right]^{1/2} . \tag{17}$$

In the expression (17) the integration variables have been transformed as $\pi v_j / L = \theta_j$. The numerical evaluation of (15) resulted in

$$U_{\mathrm{I}}^* = 0.5230 \pm 0.0012 \tag{18}$$

where the error is due to the numerical integration.

Secondly, we consider the Gaussian model, for which the central charge is unity, $c = 1$. The Gaussian model has an infinite number of the scaling fields $\{S_{n,m}\}$. The multipoint correlation functions on the infinite plain are given by the general formula [16]:

$$\left\langle \prod_{j=1}^{N} S_{n_j,m_j}(z_j) \right\rangle_{\text{plain}} = \prod_{1 \leqslant j < k \leqslant N} z_{jk}^{\frac{1}{2}n_j^+ n_k^+} \bar{z}_{jk}^{\frac{1}{2}n_j^- n_k^-} e^{i\pi(n_j m_k - n_k m_j)/2} \tag{19}$$

where

$$n_j^{\pm} \equiv n_j\sqrt{x_p} \pm m_j/\sqrt{x_p} \tag{20}$$

with x_p depending on model parameters. In addition, the correlations (19) vanish unless the following 'charge neutrality' condition is satisfied:

$$\sum_{j=1}^{N} n_j = \sum_{j=1}^{N} m_j = 0\,. \tag{21}$$

If the order-parameter operator $\mathcal{O}$ contains the combination of the scaling fields $S_{n,m} + S_{-n,-m}$, we have the two-point function in the form

$$\begin{aligned}\langle \mathcal{O}(z_1)\mathcal{O}(z_2)\rangle_{\text{plain}} &= \frac{A^2}{2}\left(\langle S_{n,m}S_{-n,-m}\rangle_{\text{plain}} + \langle S_{-n,-m}S_{n,m}\rangle_{\text{plain}}\right) \\ &= \frac{A^2}{|z_{12}|^{\eta}}\end{aligned} \tag{22}$$

where

$$\eta \equiv n^2 x_p + m^2/x_p\,. \tag{23}$$

Here we have focused on the spinless case $nm = 0$. Similarly, the four-point function is given by

$$\langle \mathcal{O}(z_1)\mathcal{O}(z_2)\mathcal{O}(z_3)\mathcal{O}(z_4)\rangle_{\text{plain}} = \frac{A^4}{2}\left[\left|\frac{z_{12}z_{34}}{z_{13}z_{14}z_{23}z_{24}}\right|^{\eta} + (2 \leftrightarrow 3) + (2 \leftrightarrow 4)\right]. \tag{24}$$

The same procedure as (11)–(14) gives the critical-point Binder parameter (2) for the Gaussian universality class in the following form:

$$U_G^* = 1 - \frac{1}{6\pi^2}\frac{b_G}{a_G^2} \qquad \text{for} \quad c = 1 \tag{25}$$

with

$$a_G \equiv \frac{\Gamma((1-\eta)/2)}{\Gamma(1-\eta/2)} \tag{26}$$

and

$$b_G \equiv \iiint_0^{\pi} d\theta_2 d\theta_3 d\theta_4 \left[\left|\frac{s_{12}s_{34}}{s_{13}s_{14}s_{23}s_{24}}\right|^{\eta} + (2 \leftrightarrow 3) + (2 \leftrightarrow 4)\right]. \tag{27}$$

It is easy to see that we have $U_G^*(\eta = 0) = \frac{1}{2}$. The Taylor expansion with respect to η gives

$$U_G^* = \tfrac{1}{2} + O(\eta^2)\,. \tag{28}$$

We show in figure 1 the numerical estimates of (25) for larger η. The change with respect to η is monotonic. The value for $\eta = \frac{1}{4}$ was estimated at

$$U_G^*(\eta = \tfrac{1}{4}) = 0.4553 \pm 0.0014\,. \tag{29}$$

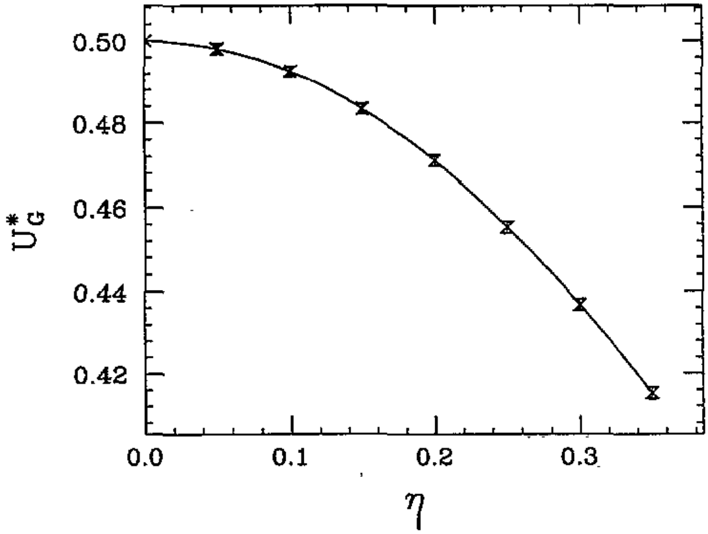

Figure 1. The η-dependence of the critical-point Binder parameter for $c = 1$. The errors of the estimates are due to the numerical integration. The line is a guide for the eye.

Let us describe an example in which we actually observed the above estimates, and discuss their finite-size corrections. We treated the $S = 1$ antiferromagnetic XXZ model in one dimension:

$$\mathcal{H} \equiv \sum_{i=1}^{L} \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z \right] \tag{30}$$

with the periodic boundary condition $\vec{S}_{L+1} = \vec{S}_1$. We numerically diagonalized the Hamiltonian by the Lanczos method [26] for $L \leqslant 16$.

The model has been studied extensively since Haldane conjectured [17, 18] that the ground state is disordered at the Heisenberg point $\lambda = 1$. After detailed numerical studies [19–25], it is known that there are two phase transitions at $\lambda_c \simeq 1.2$ (between the Néel phase and the Haldane phase) and at $\lambda_c \simeq 0$ (between the Haldane phase and the XY phase). The first one is probably of the two-dimensional Ising universality class, i.e. $c = \frac{1}{2}$. The second one is thought to be of the Kosterlitz–Thouless type, i.e. $c = 1$, and hence the XY phase to be the massless Gaussian phase.

First we explain the results for the transition between the Néel phase and the Haldane phase. The order-parameter operator for the Néel phase is given by the staggered magnetization,

$$\mathcal{O}_i = (-1)^i S_i^z \,. \tag{31}$$

The scaling dimension of the operator $\mathcal{O}_i$ is expected to be $\frac{1}{2}\eta = \frac{1}{8}$.

Varying the anisotropy λ, we estimated the crossing point $(\lambda_c(L, L+2), U^*(L, L+2))$ of the equal-time Binder parameters $U(\lambda; L)$ and $U(\lambda; L+2)$. In our previous study [25] we analysed the data allowing for the logarithmic correction, and thus obtained the estimate $U^* = 0.544(4)$. After knowing the value (18) we have become aware that the correction is more modest, namely of the order L^{-2}; assuming this correction we observe the convergence to the value (18) as is shown in figure 2. The information about the form of the correction enables us to extrapolate accurately the critical-point estimate λ_c from the data $\lambda_c(L, L+2)$.

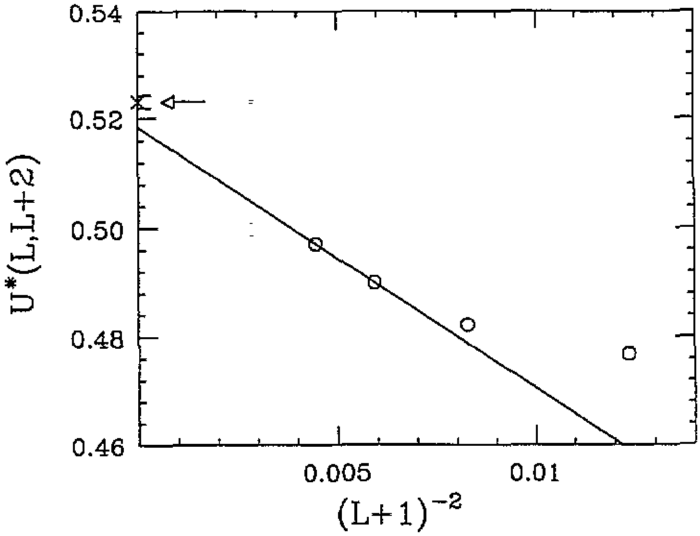

Figure 2. The values of the Binder parameter at the crossing points of $U(\lambda; L)$ and $U(\lambda; L+2)$. These are based on the data for $8 \leqslant L \leqslant 16$ near $\lambda \simeq 1.2$, or the boundary between the Néel phase and the Haldane phase. We joined the last two data points to draw the full line. The symbol on the ordinate indicates the prediction (18).

Thus we obtained

$$\lambda_c = 1.186 \pm 0.002\,. \tag{32}$$

This is consistent with the result of an earlier study [24].

Note that the correction to finite-size scaling of the energy gap is expected to be of the order L^{-1} [12]. The reduction of the correction of the Binder parameter to the order L^{-2} may result from some cancellation due to the division in the definition of the Binder parameter (1).

Next we explain our analysis at $\lambda = 0$. The 'pseudo' order-parameter operator [27] for the XY phase may be given by

$$\mathcal{O}_i = S_i^x = \tfrac{1}{2}(S_i^+ + S_i^-) \tag{33}$$

though the order does not emerge because of the continuous criticality in the XY phase. The operators $S_i^{\pm}$ are expected [28] to correspond to the scaling fields $S_{\pm 1,0}$, and hence the correlation exponent η in (23) is reduced to $\eta = x_{\mathrm{p}}$.

So far the location of the transition point between the Haldane phase and the XY phase has been controversial [19–22, 24, 29]. Alcaraz and Moreo [30] conjectured that the exponent η at the anisotropy λ should be given by the following formula if the point of the anisotropy is located inside the XY phase:

$$\eta = x_{\mathrm{p}} = \frac{\pi - \cos^{-1}\lambda}{2\pi} \qquad \text{for} \quad \lambda \leqslant \lambda_c\,. \tag{34}$$

According to this conjecture we have $\eta = \frac{1}{4}$ for $\lambda = 0$.

We evaluated the equal-time Binder parameter (1) at $\lambda = 0$ for $L \leqslant 16$. When we allowed for the logarithmic correction [31], the estimate extrapolated from our data was $U^* = 0.436 \pm 0.004$, which is inconsistent with the value for $\eta = \frac{1}{4}$, (29). When we assumed the leading correction to be of the order L^{-1} instead, we extrapolated the estimate

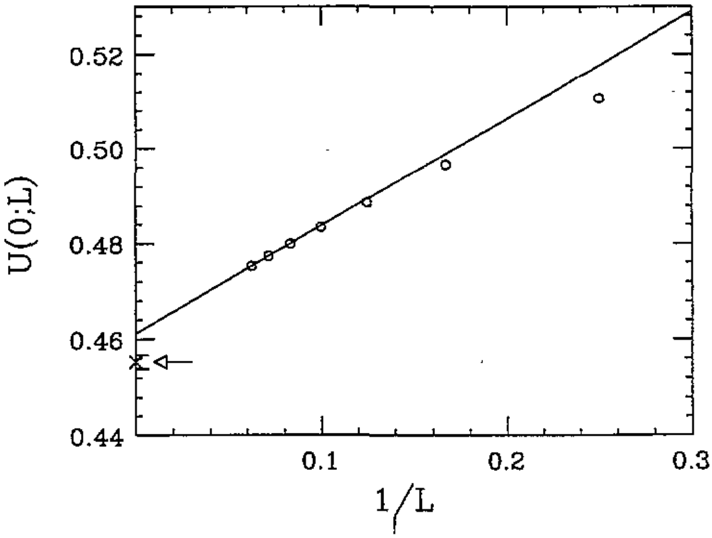

Figure 3. The L-dependence of the Binder parameter at $\lambda = 0$. We joined the last two data points for $L = 14$ and $L = 16$ to draw the full line. The symbol on the ordinate indicates the prediction (29).

$U^* = 0.462 \pm 0.004$ as is shown in figure 3; this estimate agrees with the value (29). Considering the above analysis of the transition at $\lambda \simeq 1.2$, it is possible that the order of the correction again becomes higher with respect to L^{-1}.

To summarize, we evaluated the universal values of the equal-time Binder parameter for $c = \frac{1}{2}$ and $c = 1$ with the help of the conformal field theory. We compared the values with the results of the numerical-diagonalization study of the $S = 1$ antiferromagnetic XXZ chain. We found that the correction terms may be of a higher order in L^{-1} than expected.

Acknowledgments

The present author is grateful to Mr K Totsuka for helpful discussions. The numerical calculations are supported by Grant-in-Aid for Scientific Research on Priority Areas 'Computational Physics as a New Frontier in Condensed Matter Research', from the Ministry of Education, Science and Culture, Japan.

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