Test of modular invariance for finite XXZ chains

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Abstract. The central charge c of the Virasoro algebra is determined using its relation to the set of anomalous dimensions of the scaling fields for the critical anisotropic Heisenberg chain. The results obtained by exactly solving the Bethe ansatz for $N \leq 4$ are compared with the standard procedure of calculating c in the whole region of anisotropy. For odd N the system is no longer modular invariant and the analogous averaging leads to an anisotropy-dependent function which has been calculated.

1. Introduction

Two dimensional conformally invariant systems of statistical mechanics (e.g. 6-vertex-models) are characterized by their central charge c and a set of operator dimensions $\{x_n\}$, the eigenvalues of the dilatation generator $L_0 + \bar{L}_0$ of the corresponding Virasoro algebras with central charge c. Consider now the partition function $Z = \mathrm{Tr}\, \mathrm{e}^{-\beta H}$ of a one-dimensional quantum system of length N (e.g. the anisotropic Heisenberg model XXZ). In the limit $\beta \to \infty$ this expression can be viewed as the partition function of a strip of infinite length and finite width N. For periodic boundary conditions, which are assumed throughout the paper, this corresponds to a cylinder in space direction N. It follows now that at criticality for large N the Hamiltonian H of the quantum system can be mapped according to

$$H \to \frac{2\pi v}{N}\left(L_0 + \bar{L}_0 - \frac{c}{12}\right) \tag{1.1}$$

The parameter v is an effective velocity rescaling the energy and can be analytically determined by a low-energy dispersion relation. The low-energy excitations are (in leading orders) completely given through c and $\{x_n\}$:

$$\Delta E_0^{(N)} = E_0^{(N)} - E_0^{(\infty)} = -\frac{c\pi v}{6N} \tag{1.2}$$

$$E_n^{(N)} - E_0^{(N)} = \frac{2\pi v}{N} x_n \tag{1.3}$$

Here $E_0^{(N)}$ is the ground state energy and $E_n^{(N)}$ stands for the energy of an excited state both with N sites. $E_0^{(\infty)}$ is the leading part (proportional to N) of the ground state energy for $N \to \infty$ (Affleck 1986, Blöte *et al* 1986).

The standard way of calculating the central charge c of a given system is via relation (1.2) which requires the exact ground state energy $E_0^{(N)}$ for moderately large values of N.

It is straightforward to obtain c using the information of the whole spectrum of H expecting better results for smaller N than above.

An important step in this direction has been made by Schütz (1992) for modular invariant systems. He derived a relation between c and $\{x_n\}$

$$c = 12 \frac{\sum_n x_n \exp(-2\pi x_n)}{\sum_n \exp(-2\pi x_n)} \tag{1.4}$$

and checked for Ising and other models. Also comparing the standard way of calculating c (equation (1.2)) and its calculation via equations (1.4) and (1.3) through the knowledge of the whole excitation spectrum, Schütz (1992) found that the latter works better starting with $N \approx 4$. Of course there is no guarantee that this fact holds for other models. It seems now worthwhile testing relation (1.4) for models with a critical region where the $\{x_n\}$ depend on an additional parameter ('coupling constant') while c is a constant in the whole region. This has been done in the present paper for XXZ model and $N = 2, 4$. The spectrum of the Hamiltonian can be determined analytically by the Bethe ansatz. The results for $N = 4$ are presented in detail in section 2. In section 3 we compare the results for c in case of even N, while section 4 is devoted to $N = 3$, where modular invariance for our boundary conditions is no longer valid. Section 5 contains our conclusions.

2. Anisotropic Heisenber model with $N=4$

For definiteness we use the Hamiltonian

$$H = \frac{1}{4} \sum_{n=1}^{N} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta(\sigma_n^z \sigma_{n+1}^z - 1)] \tag{2.1}$$

with $\Delta = \cos\gamma$ and $0 \leqslant \gamma$ and $0 \leqslant \gamma < \pi$.

To obtain the spectrum of H one has to solve the Bethe ansatz equations

$$\left(\frac{\sinh\left(\lambda_j + \frac{i\gamma}{2}\right)}{\sinh\left(\lambda_j - \frac{i\gamma}{2}\right)} \right)^N = \prod_{k=1, k \neq j}^{l} \frac{\sinh(\lambda_j - \lambda_k + i\gamma)}{\sinh(\lambda_j - \lambda_k - i\gamma)} \qquad j = 1, \dots, l \tag{2.2}$$

for $l \leqslant \frac{1}{2}N$. Any of its solutions $\lambda_j \neq \lambda_k$ for $j \neq k$ corresponds to an eigenstate with

$$E = \sum_{j=1}^{l} \frac{-\sin^2\gamma}{\cosh(2\lambda_j) - \cos\gamma} \qquad P = \frac{1}{i} \sum_{j=1}^{l} \ln\left(\frac{\sinh\left(\lambda_j + \frac{i\gamma}{2}\right)}{\sinh\left(\lambda_j - \frac{i\gamma}{2}\right)} \right) \qquad S_z = \frac{N}{2} - l.$$

Table 1. The eigenstates of the XXZ Hamiltonian with $N=4$ calcualted via the Bethe ansatz technique. Bethe ansatz roots, energy, momentum and spin are shown.

State	$\{\lambda\}$		E	P	$\|S_z\|$	S
1	$\pm\coth^{-1}\left(\dfrac{3+(8+\cos^2\gamma)^{1/2}}{1-\cos\gamma}\right)^{1/2}$		$-2(\Delta+1)\dfrac{\Delta+2+(\Delta^2+8)^{1/2}}{\Delta+4+(\Delta^2+8)^{1/2}}$	0	0	0
2	$\pm\dfrac{i\gamma}{2}$		$-\Delta$	π	0	0
3	0	$\dfrac{i\pi}{2}$	-2Δ	π	0	1
4, 5	x	$-x+\dfrac{i\pi}{2}$	$-\Delta$	$\pm\dfrac{\pi}{2}$	0	1
	$x=\pm\tanh^{-1}\dfrac{1-(1+\sin^2\gamma)^{1/2}}{\sin\gamma}$					
6	$x+\dfrac{i\pi}{2}$	$-x+\dfrac{i\pi}{2}$	$-2(\Delta+1)\dfrac{\Delta+2-(\Delta^2+8)^{1/2}}{\Delta+4-(\Delta^2+8)^{1/2}}$	0	0	2
	$x=\tanh^{-1}\left(\dfrac{3-(8+\cos^2\gamma)^{1/2}}{1-\cos\gamma}\right)^{1/2}$					
7, 8	$\dfrac{i\pi}{2}$		$1-\Delta$	0	1	2
9, 10	0		$-(1+\Delta)$	π	1	1
11, 12 13, 14	$\pm\tanh^{-1}\left(\tan\dfrac{\gamma}{2}\right)$ $\quad 0\le\gamma\le$		$-\Delta$	$\pm\dfrac{\pi}{2}$	1	1
	$\dfrac{\pi}{2}$					
	$\pm\coth^{-1}\left(\tan\dfrac{\gamma}{2}\right)$ $\quad \dfrac{\pi}{2}\le\gamma\le$					
	π					
15, 16	no λ		0	0	2	2

$|\mathrm{Im}\,\lambda|$ has to be restricted to being smaller than $\frac{1}{2}\pi$ and $\mathrm{Im}\,\lambda=\frac{1}{2}\pi$ must be set equivalent to $\mathrm{Im}\,\lambda=-\frac{1}{2}\pi$. The states with $S_z<0$ are produced just by counting any state with $S_z>0$ twice.

The results of our calculation which, of course, may have been done earlier, are shown in table 1.

In the last column of table 1 we attached a quantum number S to any state, obtained by continuing from $\Delta=1$ (XXX model) where this number is conserved. The results for $\gamma=0$ are given after the usual limiting procedure including the rescaling of λ by γ^{-1} whereafter all states with $\mathrm{Im}\,\lambda=\frac{1}{2}\pi$ disappear. This is in full agreement with the Bethe ansatz for XXX which gives the highest weights states only.

The energies of all states are shown in figure 1, which shows the well known central symmetry with respect to the point $\Delta=0$. The accidental degeneration of the states 2, 4 and 11 is due to the small N. States 4 and 11 represent two triplets. The typical situation of such multiplets is given for the third triplet (states 3 and 9) and the pentuplet (states 6, 7 and 15), where all members cross at $\Delta=1$.

For $\Delta\ge 1$ the (antiferromagnetic) ground state is a singlet (1), while for $\Delta\le-1$ the two (ferromagnetic) ground states are states 15 and 16 (highest members of the pentuplet).

It is interesting to look for the Bethe ansatz solution in the region $|\Delta| > 1$, too. One can easily see that using the parameterization $\Delta = \text{sgn}\,\Delta \cosh \bar{\gamma}$ the new solutions are obtained from those of table 1 by the replacement $\bar{\lambda} = -\,\mathrm{i}\cdot\lambda(\mathrm{i}\cdot\bar{\gamma})$.

An effect worth mentioning occurs only for the two states 4 and 5. Taking for definiteness the sign plus for x in table 1 both $\bar{\lambda}$ stay real as long as $\sinh(\bar{\gamma}) \leqslant 1$ and coalesce at $x = \frac{1}{4}\pi$ for $\sinh \bar{\gamma} = 1$: For larger $\bar{\gamma}$ they acquire imaginary parts of different signs $\operatorname{Im} \bar{\lambda} = \pm[\cosh^{-1}(\sinh \bar{\gamma})]/2$ preserving their real parts. We have checked that throughout the whole region of Δ the energies of table 1 are correct as they are written as functions of Δ only.

3. Calculation of central charge for $N=2$ and $N=4$

With the results of section 2 we can now calculate c via equations (1.3) and (1.4). Before doing so we demonstrate how equation (1.4) works if the exact dimensions are used. The set of primary operators is given through

$$x_{n,m} = \frac{n^2}{2}(1-\nu) + \frac{m^2}{2(1-\nu)} \tag{3.1}$$

by Alcaraz *et al* (1988a) where for even N, n and m are integers. Parameter ν is defined through $\nu = \gamma/\pi$. We shall consider only primary and secondary operators with $x_n \leqslant 2$.

For $\nu = 0$ we have the following primary operators (in brackets their multiplicity is indicated): $0(1)$, $\frac{1}{2}(4)$, $1(4)$, $2(4)$ leading to $c = 0.954\,900$. Including the secondary operators $1(2)$, $\frac{3}{2}(8)$, $2(13)$ gives $c = 0.999\,889$.

For $\nu = \frac{1}{2}$ ($\Delta = 0$) one has: $0(1)$, $\frac{1}{4}(2)$, $1(4)$, $\frac{9}{4}(4)$, $2(4)$ for the primary operators and $c = 0.954\,902$. Including $1(2)$, $\frac{5}{4}(4)$, $2(13)$ gives $c = 0.999\,728$.

Approaching $\nu \to 1$ one has to take into account an infinite set of primary operators. We therefore expect troubles for finite N if $\gamma \to \pi - \varepsilon$. From a physical point
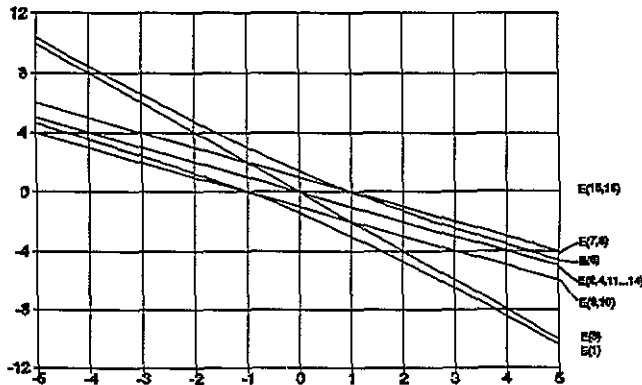

Figure 1. The energies of all eigenstates of XXZ Hamiltonian with $N=4$ sites calculated via the Bethe ansatz technique. For the classification of the eigenstates see table 1.
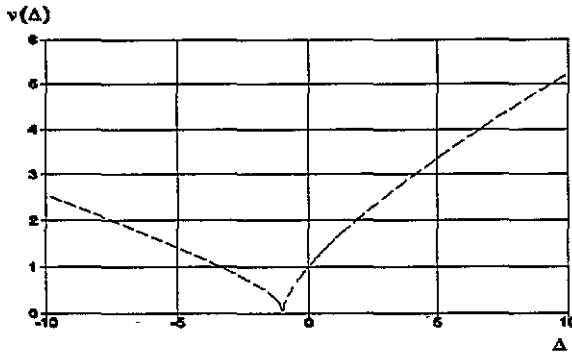
v(Δ)

Figure 2. The effective velocity $v = (\pi/2)(\sin \gamma/\gamma)$ as a function of the anisotropy para-meter Δ continued to non-critical values of $|\Delta| > 1$. The edge singularity is located at $\Delta = -1$.

of view (phase transition antiferromagnetic/ferromagnetic) this is no surprise, of course.

In the paper of Schütz (1992) it has been mentioned that it is useful to consider the weighted average $\langle x_n \rangle$ for arbitrary Δ. The only problem to overcome then is caused by the appearance of the parameter v in equation (1.3). For $|\Delta| < 1$ one has

$$v = \frac{\sin(\gamma)}{\gamma} \frac{\pi}{2}. \tag{3.2}$$

It is straightforward to assume for $\Delta > 1$

$$v = \frac{\sinh(\tilde{\gamma})}{\tilde{\gamma}} \frac{\pi}{2} \tag{3.3}$$

while for $\Delta < -1$ the continuation is not quite clear. We therefore have adopted

$$v = \frac{\sinh(\tilde{\gamma})}{(\tilde{\gamma} + \pi)} \frac{\pi}{2} \tag{3.4}$$

(remember $\Delta = -\cosh \tilde{\gamma}$). The function $v(\Delta)$ is now continuous at $\Delta = -1$ but has still a singularity which seems to be unavoidable, as oen can see from figure 2.

Replacing in the denominator of formula (3.4) $\tilde{\gamma} + \pi$ by $\tilde{\gamma}$ would lead to a drastic change of the resulting central charge in the region $\Delta \leqslant -1$. On the other hand one has to keep in mind that any method for calculating c via finite size data fails near the singularity point $\Delta = -1$ (in contrast to the other singularity at $\Delta = 1$).

Our numerical results for $N = 2$ and 4 are given in table 2 and figures 3, 4, 5 and 6. They are compared with the result of the standard procedure for determining c by finite-size corrections using equation (1.2). For those functions we have extended equation (1.2) for $\Delta > 1$. For $\Delta < -1$ one obtains a 'central charge' identical to zero. To distinguish both functions we call the first one c_a (a for average value) and the latter c_v (v for vacuum state).

Table 2. The calculation of the central charge for the XXZ equation (1.4) (second and third column) and equation (1.2) (fourth and fifth column) as function of Δ.

Δ	c_a $N=2$	c_a $N=4$	c_v $N=2$	c_v $N=4$
1	0.925 655	1.246 739	1.492 387	1.106 130
$\dfrac{(3)^{1/2}}{2}$	0.925 333	1.243 873	1.490 873	1.104 848
$\dfrac{(2)^{1/2}}{2}$	0.924 120	1.233 302	1.485 095	1.101 275
$\tfrac{1}{2}$	0.921 256	1.209 255	1.470 210	1.094 664
0	0.091 643	1.120 454	1.388 010	1.076 962
$-\tfrac{1}{2}$	0.989 731	1.014 521	1.181 825	1.035 786
$-\dfrac{(2)^{1/2}}{2}$	0.870 581	0.975 164	1.006 151	0.966 450
$-\dfrac{(3)^{1/2}}{2}$	0.767 916	0.927 682	0.763 649	0.814 525

Comparing figures 2 and 3 with the exact value $c=1$ ($|\Delta|<-1$) one can see that (1.4) already works qualitatively well for $N=2$, the improvement for $N=4$ is not so significant. Both functions show a similar behaviour (for $\Delta \geqslant -1$). Therefore one cannot say that formula (1.4) works better than (1.2) for $N=4$ as in case of the Ising model. There is still the possibility that it does so in some small region (or even in one point) of Δ. Our data suggest that this may happen in the vicinity of point $\Delta = -\sqrt{2}/2$ (Ising model). The asymptotic of $\Delta \to -1$ are all of the form $c \sim (\Delta+1)^{1/2}$. The coefficient does not only depend on N but is different for different ways of calculating c. This is not surprising because in one case it depends on all energies which states
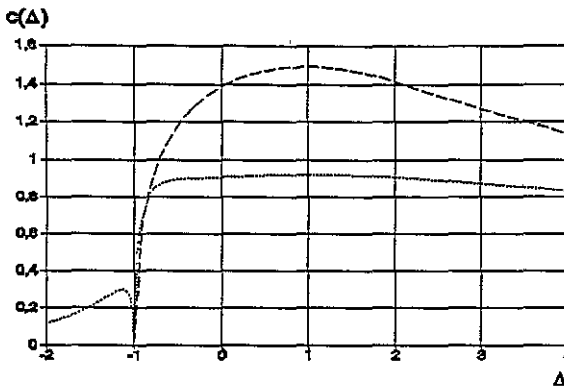

Figure 3. The finite-size determination of central charge c of XXZ model as functions of the anisotropy parameter Δ for $N=2$. The dotted curve corresponds to c_a, calculated using the Virial theorem while the dashed curve corresponds to c_v calculated using correction to vacuum energy.
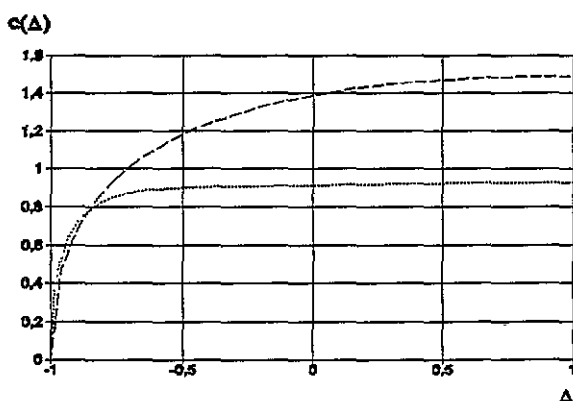
c(Δ)

Figure 4. The same as figure 3 on a larger scale.

cross at $\Delta = -1$ and in the other, on $E_0^{(\infty)}$. For $\Delta \to \infty$ the asymptotics coincide for $N = 2$ and 4 separately:

$$c^{(2)} \approx \frac{24}{\pi^2} \frac{\ln \Delta}{\Delta}$$

and

$$c^{(4)} \approx \frac{48}{\pi^2} \frac{\ln \Delta}{\Delta^2}$$

(Besides the ground state energy E_1 it depends either on E_3 or on $E_0^{(\infty)}$.) We were not able to prove that this fact is not an accident.

In the region $\Delta < -1$ figures 3 and 5 show a maximum for c_a which one should consider to be spurious. For increasing N it becomes sharper and moves towards the singularity at $\Delta = -1$. The asymptotics for $\Delta \to -\infty$ are not connected with the particular choice of formula (3.4), c_a vanishes faster (we found $c \approx \ln(-\Delta) * (-\Delta)^{-2N/\pi}$) than in the case $\Delta \to \infty$. We suggest that for $N = \infty$ the
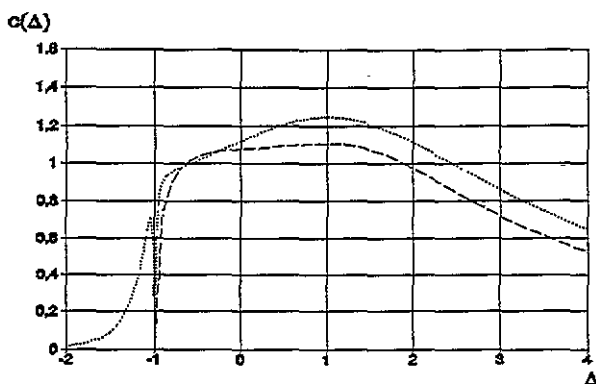
c(Δ)

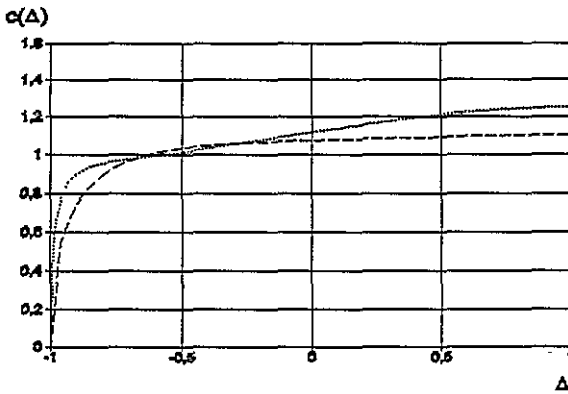**Figure 5.** The same as figure 3 for $N = 4$.

Figure 6. The same as figure 5 on a larger scale.

singularity is of the form that c goes from zero to one immediately when passing this point from left to right. On the other hand we expect c to stay smooth at the point $\Delta = 1$ $(N = \infty)$.

4. The case of odd N

It is well known that for odd N no ground state exists, an independent determination of c via (1.2) therefore must fail.

On the other hand (1.4) cannot be used, either. This is due to the fact, that modular invariance is no longer valid in this case. The set of $\{x_n\}$ is still given by formula (3.1) with both n and m half-integers. Transforming the two-dimensional partition function in the usual way one would obtain a sign factor $(-1)^n(-1)^m$ excluding modular invariance. (Modular invariance can be maintained if antiperiodic boundary conditions are introduced. The picture is still more complicated because of the sign factors. We intend to study this in a further work).

Nevertheless, it seems worthwhile demonstrating the consequences of the non-validity of modular invariance for odd N. We therefore have calculated the RHS of (1.4) throughout the critical region for $N = 3$ but this is no longer expected to equal the central charge c. We for this reason introduce the new notation $d(\Delta)$. Equation (3.1) gives the operator dimensions with respect to the 'true' ground state. We therefore have used as ground state energy

$$E_0^{(3)} = \tfrac{3}{4}E_0^{(2)} + \tfrac{3}{8}E_0^{(4)}$$

that is the average energy of the two neighbouring ground states for even N.

The exact function $d(\Delta)$ can be obtained directly via (3.1), the result is called d_t (t is for theoretical). On the other hand this compares with the result of our finite-size data via formula (1.3) called d_e (e for experimental) for $N = 3$. d_e has to approach d_t in the thermodynamic limit.

For the sake of clearness we briefly summarize the picture of states after having solved the Bethe ansatz equations. There is a quartet consisting of two states with $\lambda = \tfrac{1}{2}i\pi(E = 1 - \Delta)$ and two ferromagnetic ground states. The state with lowest energy

Table 3. The calculation of the analogue of the central charge d_e for $N=3$ compared with the theoretical value d_t (second and third column) compared with the finite-size corrections to the one-hole-state c_{1e} and c_{1t} (fourth and fifth column) as functions of Δ.

Δ	d_e	d_t	c_{1e}	c_{1t}
1	4.398 533	3.089 804	2.113 549	2
$\frac{1}{2}(3)^{1/2}$	4.402 674	3.155 656	2.119 240	2.05
$\frac{1}{2}(2)^{1/2}$	4.420 179	3.253 896	2.142 355	2.125
$\frac{1}{2}$	4.449 977	3.416 107	2.205 315	2.25
0	4.799 797	4.045 068	2.606 555	2.75
$-\frac{1}{2}$	5.582 028	5.502 904	3.956 840	4
$-\frac{1}{2}(2)^{1/2}$	5.357 690	7.001 165	5.593 247	5.375
$-\frac{1}{2}(3)^{1/2}$	3.550 148	9.999 998	9.110 045	8.25

is four times degenerated (2 doublets) with $E = -\frac{1}{2}(1+2\Delta)$ (1-hole state). It corresponds to the two solutions

$$\lambda = \pm \tanh^{-1}\left(\frac{\tan(\gamma/2)}{\sqrt{3}}\right) \qquad \text{for } 0 < \gamma < \frac{2\pi}{3}$$

and

$$\lambda = \pm \tanh^{-1}\left(\sqrt{3}\cot\frac{\gamma}{2}\right) \qquad \text{for } \frac{2\pi}{3} < \gamma < \pi.$$

The energy is given by the same function as above. Results are presented in table 3 and figures 7 and 8.

Numerical calculations have shown that the inclusion of the secondary operators shifts d by a constant
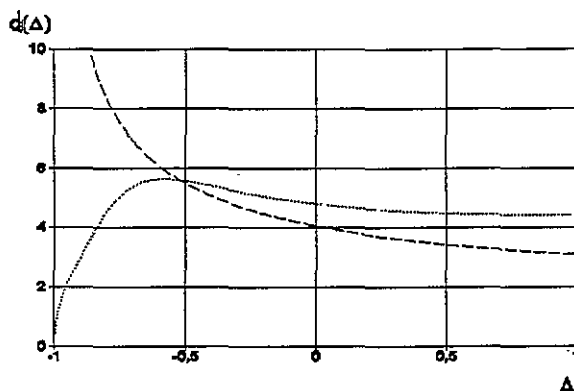
$$\Delta d = 0.045068$$

Figure 7. The analogue of the central charge in case of odd N as function of the anisotropy parameter Δ for $N=3$ given by the dotted curve. The dashed curve corresponds to its theoretical value for $N \to \infty$ calculated by summing up the exact operator dimensions.
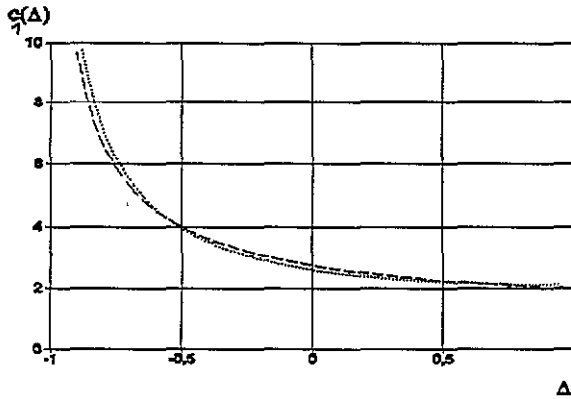
Figure 8. The comparison of the finite-size correction to the first excited state for $N=3$ (dotted curve) to its theoretical value (dashed curve) as fuction of Δ.

(This effect is already included in the presented data.) The two curves in figure 7 show only a slight coincidence. The different behaviour near the point $\Delta \rightarrow -1$ is not so surprising, d_e shows the same singularity ($\approx (\Delta+1)^{1/2}$) as for even N (see above). In the other region the difference between d_e and d_t is significantly higher than for $N=2$ which we understand as a hint for a hidden compensation mechanism working only for the 'true' central charge. A further test is possible where a modified version of (1.2) is used. For odd N we put in $E_1^{(N)}$ instead of $E_0^{(N)}$, the energy of the lowest state (1 hole) and omit the sign $-$. The resulting 'c' we call c_{1e}, being compared with its theoretical value for large N, c_{1t}

$$c_{1t} = \frac{1}{2} - \frac{2}{3} \nu + \frac{3}{2(1-\nu)} \tag{4.1}$$

according to standard philosophy by Woynarovich (1987). The results are included in table 3 and figure 8.

We are surprised by the strikingly good agreement between c_{1e} and c_{1t}, which is even better than the corresponding data for $N=4$ (table 2). Near $\Delta \rightarrow -1$ they show qualitatively the same behaviour ($\approx (\Delta+1)^{-1/2}$) but the coefficients are different.

We cannot explain why our results for c_1 do not fit with those of Alcaraz *et al* (1988b) (see e.g. formula (3.22)). On the other hand they fit very well in the isotropic case with the numerical data of Fabricius *et al* (1991).

5. Conclusions

On the basis of our results we can state that the method of Schütz works in the case of the XXZ model considered above. The aim of obtaining better numerical coincidence for very small N compared to the standard method of calculating c could not be verified in general. Our results clearly show that one may expect such an effect only in some parts of the whole critical region. Because those parts are not known *a priori* this fact is of no great use for practical calculations. The method definitely fails near the phase transition point $\Delta = -1$ but works well near the Kosterlitz–Thouless point $\Delta = 1$ which fits well with standard knowledge.

Comparing the results of both methods for $N=2$ and $N=4$ for arbitrary anisotropy we find it most remarkable that the basic physical effects of the system are reflected in our curves. We here have in mind especially the smooth transition at the Kosterlitz–Thouless point and the singularity at the phase transition point. This leads us to the conclusion that combining just two independent methods one obtains a lot of physical important information from a very small number of sites. We believe that this is due to the high symmetry of the model (conformal and modular). To obtain more information on that fundamental fact one has to consider correction terms and to clarify compensation mechanisms.

The case of odd N is helpful in preventing too far-reaching speculations. The loss of modular invariance drastically changes the picture. No physical reliable information can be obtained from the function $d(\Delta)$, which is a clear signal to be careful with general consequences. We wish to stress that some features of the system with an odd number of sites are still correctly reproduced with $N=3$ sites. This has been demonstrated for example, for the energy of the 1-hole-state.

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