Corrections to finite-size scaling for quantum chains

1984 J. Phys. A: Math. Gen. 17 L469

(http://iopscience.iop.org/0305-4470/17/9/003)

J. Phys. A: Math. Gen. 17 (1984) L469–L472. Printed in Great Britain

LETTER TO THE EDITOR

Corrections to finite-size scaling for quantum chains

G V Gehlen, C Hoeger and V Rittenberg
Physikalisches Institut, Universität Bonn, Nussallee 12, 5300 Bonn, West Germany

Received 26 March 1984

Abstract. We compute the leading order correction to the energy gap at the critical point for the anisotropic Ising and the Z_3 Potts quantum chains. Periodic, anti-periodic and free boundary conditions are considered. For the Ising case the corrections are independent of the boundary conditions. In the Z_3 case the correction is the same for anti-periodic and free boundary conditions but is $\frac{2}{5}$ smaller for the periodic case. We have no explanation for this phenomenon.

Derrida and de Seze (1982) and Luck (1982) have considered two-dimensional lattices with isotropic interactions, infinite in the first direction and of finite size N in the second one. They have suggested that if one studies the behaviour at large N of the correlation length ξ_N in the infinite direction at the critical point T_c,

$$\xi_N(T_c) = A_0 N(1 + A_1 N^{-\sigma} + \ldots) \tag{1}$$

the coefficient A_0 should have a physical meaning:

$$A_0 = 1/\pi\eta \tag{2}$$

where η is the critical exponent describing the anomalous dimension of the spin–spin correlation at the critical point. This idea was further extended by Nightingale and Blöte (1983) to anisotropic systems.

In this letter we ask a similar question concerning quantum chains, motivated by the fact that performing an anisotropic limit of $\infty \times N$-site two-dimensional spin systems leads to N-site quantum chains (Fradkin and Susskind 1978). Then the energy gap of the quantum chain (the difference between the two lowest energy eigenvalues) corresponds to ξ_N^{-1} of equation (1). Quantum chains have also attracted considerable interest themselves, see e.g. Barouch and McCoy (1971a, b).

We consider a Hamiltonian $H(\lambda)$ with N sites depending on a parameter λ such that for $N \to \infty$ the energy gap vanishes at $\lambda = \lambda_{cr}$. In analogy with equation (1) for large N we may expect

$$N E_N(\lambda_{cr}) = B_0(1 + B_1 N^{-\omega} + \ldots) \tag{3}$$

with B_0 having a physical meaning. If so its value should be independent of the boundary conditions. In order to get an answer to our question we consider two examples.

We first consider the well known Hamiltonian (Katsura 1962)

$$H = -\sum_{i=1}^{N} \sigma_i^z - \lambda \sum_{i=1}^{N} [\tfrac{1}{2}(1+\gamma)\sigma_i^x \sigma_{i+1}^x + \tfrac{1}{2}(1-\gamma)\sigma_i^y \sigma_{i+1}^y] \tag{4}$$

where σ_i^x, σ_i^y, and σ_i^z are Pauli matrices. This model has for $\gamma \neq 0$ an Ising type phase transition at $\lambda = 1$. We take three types of boundary conditions: (A) periodic, (B) anti-periodic, and (C) free. The analytic result for cases (A) and (B) has been given by Katsura (1962, equations (2.26), (2.27)):

$$NE_N^{(A)}(\lambda = 1) = N \sum_{k=0}^{N-1} (\Lambda(k+\tfrac{1}{2}) - \Lambda(k)) \tag{5}$$

$$NE_N^{(B)}(\lambda = 1) = -NE_N^{(A)}(\lambda = 1) + N\Lambda(\tfrac{1}{2}) \tag{6}$$

where

$$\Lambda(k) = \{[\cos(2\pi k/N) - 1]^2 + \gamma^2 \sin^2(2\pi k/N)\}^{1/2}. \tag{7}$$

Rewriting equation (5) in the form

$$NE_N^{(A)}(\lambda = 1) = \tfrac{1}{2}N\left(\Lambda(\tfrac{1}{2}) + \Lambda(N-\tfrac{1}{2}) + \sum_{k=1}^{N-1} (\Lambda(k-\tfrac{1}{2}) + \Lambda(k+\tfrac{1}{2}) - 2\Lambda(k))\right) \tag{8}$$

and expressing the sum in equation (8) as an integral over the second derivative of Λ, we find in the leading order of N

$$NE_N^{(A)}(\lambda = 1) = NE_N^{(B)}(\lambda = 1) = \tfrac{1}{2}\gamma\pi. \tag{9}$$

For case (C) we have done the calculations numerically and the results are shown in figure 1 for three values of γ ($\gamma = 0.5$, 0.7 and 1). One sees that the values for NE_N

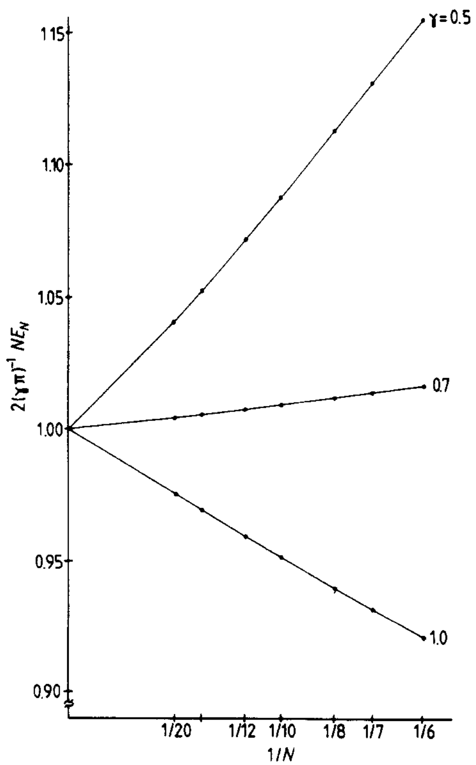

Figure 1. $2(\gamma\pi)^{-1}NE_N(\lambda = 1)$ as a function of $1/N$. $E_N(\lambda = 1)$ represents the energy gap at the critical point for the Ising Hamiltonian given by equation (4).

converge nicely to the value $\frac{1}{2}\gamma\pi$. One concludes that for the Hamiltonian given by equation (4) the finite-size scaling correction term B_0 in equation (3) is independent of the boundary conditions and might have a physical interpretation similar to equation (2) ($\eta = \frac{1}{4}$ in this case).

We now turn to a second example which is the Z_3 Potts Hamiltonian (Elitzur *et al* 1979)

$$H = \sum_{i=1}^{N} \Omega_i - \tfrac{1}{3}\lambda \sum_{i=1}^{N} (\Gamma_i \Gamma_{i+1}^{+} + \Gamma_i^{+} \Gamma_{i+1}) \tag{10}$$

where

$$\Gamma_i = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \Omega_i = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{11}$$

Here again the energy gap vanishes for $\lambda = 1$. We consider the boundary conditions: (A) periodic ($\Gamma_{N+1} = \Gamma_1$), (B) 'anti-periodic' ($\Gamma_{N+1} = e^{2\pi i/3}\Gamma_1$) and (C) free ($\Gamma_{N+1} = 0$) and naively expect the finite-size scaling correction term B_0 in equation (3) to be independent of the boundary conditions.

We have computed numerically the values of NE_N for the three cases and the values are given in table 1. To our surprise the values obtained for the periodic boundary condition (case (A)) are very different from those for the other two cases. We have estimated the limiting values of $2\pi^{-1}NE_N(\lambda = 1)$ in the three cases (we took units of $\frac{1}{2}\pi$ as suggested by equation (9)) and obtained

$$\begin{aligned} &\text{case (A)} \qquad (2/\pi)B_0 = 0.46184 \\ &\text{case (B)} \qquad (2/\pi)B_0 = 1.15469 \\ &\text{case (C)} \qquad (2/\pi)B_0 = 1.15477. \end{aligned} \tag{12}$$

The estimates were made by computing Vanden Broeck and Schwartz (1979) approximants and looking for their stability. The errors are probably in the last two

Table 1. $NE_N(\lambda = 1)$ for the Z_3 Potts Hamiltonian. The boundary conditions A, B, and C are explained in the text.

	Boundary condition		
N	A	B	C
2	0.792 789 598 33	1.516 611 48	1.281 861 05
3	0.760 314 446 41	1.637 299 79	1.411 525 68
4	0.748 391 944 85	1.688 568 25	1.486 826 19
5	0.742 441 077 65	1.716 473 91	1.536 432 61
6	0.738 937 476 31	1.733 923 41	1.571 789 61
7	0.736 649 280 47	1.745 845 80	1.598 383 15
8	0.735 044 694 98	1.754 507 16	1.619 182 15
9	0.733 859 792 71	1.761 088 19	1.635 938 77
10	0.732 949 855 33		1.649 756 46
11	0.732 229 342 56		
12	0.731 644 638 39		
13	0.731 160 515 04		

digits. The values for the last two boundary conditions coincide but they are different by a factor $\frac{2}{5}$ from the periodic boundary condition case (where $B_0 \approx \frac{1}{2}\pi\sqrt{3}\eta$; $\eta = \frac{4}{15}$ in the Z_3 case).

We have no simple explanation to this puzzle especially since it is the first time we know of when Z_2 and Z_3 symmetric systems behave in such a different way. This might be due to the existence of a zero mode in one case and the absence of zero modes in the other case.

References

Barouch E and McCoy B M 1971a *Phys. Rev.* A **3** 786
—— 1971b *Phys. Rev.* A **3** 2137
Derrida B and De Seze J 1982 *J. Physique* **43** 475
Elitzur S, Pearson R B and Shigemitsu J 1979 *Phys. Rev.* D **19** 3698
Fradkin E and Susskind L 1978 *Phys. Rev.* D **17** 2637
Hamer C J and Barber M N 1980 *J. Phys. A: Math. Gen.* **13** L169
Katsura S 1962 *Phys. Rev.* **127** 1508
Luck J M 1982 *J. Phys. A: Math. Gen.* **15** L169
Nightingale P and Blöte H 1983 *J. Phys. A: Math. Gen.* **16** L657
Vanden Broeck J-M and Schwartz L W 1979 *SIAM J. Math. Anal.* **10** 658