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LETTER TO THE EDITOR

Conformal invariance and non-universality in quantum spin chains with a defect

L G Guimarães and J R Drugowich de Felício

Departamento de Física e Ciência dos Materiais do Instituto de Física e Química de São Carlos, Universidade de São Paulo, CP 369, São Carlos, 13560, Brazil

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Abstract. We study quantum analogues of two-dimensional Ising models with a linear defect. Conformal invariance and scaling arguments are used to relate the exponent η^* (of the time correlation function of the spin at the defect) to a finite chain mass-gap ratio. Close agreement is found with the pertinent exact results.

Recently Turban (1985) has used conformal invariance and transfer matrix methods to obtain the non-universal behaviour of the spin–spin correlation function in two-dimensional Ising models with a linear defect, i.e. a line of modified nearest-neighbour couplings (see figures 1(a) and 1(b)). The attractive feature of those systems is that they are non-interacting (but defected) Fermi systems exhibiting a critical index which depends continuously on the modified coupling. Motivated by the success of the above mentioned investigation we have decided to use conformal invariance in studying time correlations in defected quantum spin chains for which analytical results can be easily worked out.

Before presenting the one-dimensional quantum models let us summarise the main results on classical two-dimensional inhomogeneous Ising models. Exact calculations (Bariev 1979, McCoy and Perk 1980) have revealed that the exponent η^* of the spin–spin correlation function (along the defect line) is given by

$$\eta^* = \left(\frac{2}{\pi}\tan^{-1} K\right)^2 \tag{1}$$

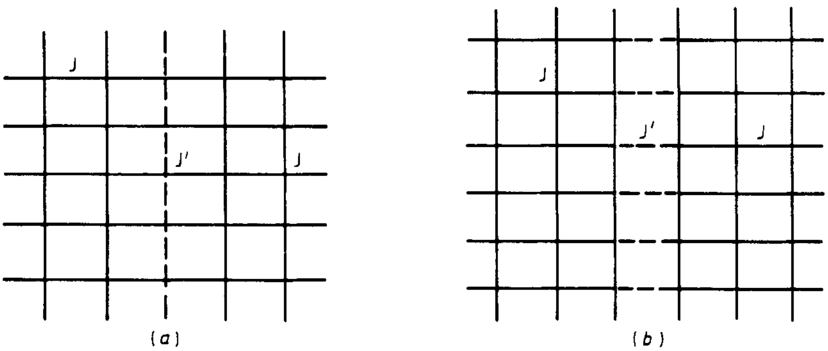

Figure 1. Ising model with a defect line: (a) the chain geometry and (b) the ladder geometry along which the strength of the interaction is modified (J'). J is the bulk interaction strength.

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where

$$K = \frac{\tanh(\beta_c J_1)}{\tanh(\beta_c J)} \qquad \beta_c = 1/kT_c \tag{2}$$

for the case of figure 1, and

$$K = \frac{\tanh(\beta_c J)}{\tanh(\beta_c J_2)} \tag{3}$$

for the ladder case (see figure 1(*b*)). In equation (2) J_1 is the dual of the modified coupling J' of figure 1(*a*)

$$\exp(-2\beta_c J_1) = \tanh(\beta_c J') \tag{4}$$

whereas J_2 in equation (3) is exactly equal to the modified coupling J' of figure 1(*b*). Equation (1) was checked by Nightingale and Blöte (1982) who calculated the defect susceptibility of finite strips to obtain γ/ν and finally η^*. As we know, usual finite-size scaling methods demand calculation of derivatives (magnetic susceptibility, for example, is the second derivative of the free energy with respect to magnetic field) which in turn requires diagonalisation of at least three Hamiltonians.

An alternative way proposed by Turban (1985) is to obtain the defect exponent η^* directly from the correlation length amplitude of a strip. In reality, this procedure is a generalisation of the remarkable universal relation between the correlation length amplitude and the bulk critical exponent η (Cardy 1984a) obtained by conformally mapping the plane onto a strip. The logarithmic mapping adequate for the strip geometry reduces the entire plane with a linear defect into a strip with two linear defects and periodic boundary conditions (figure 2). In addition, the asymptotic

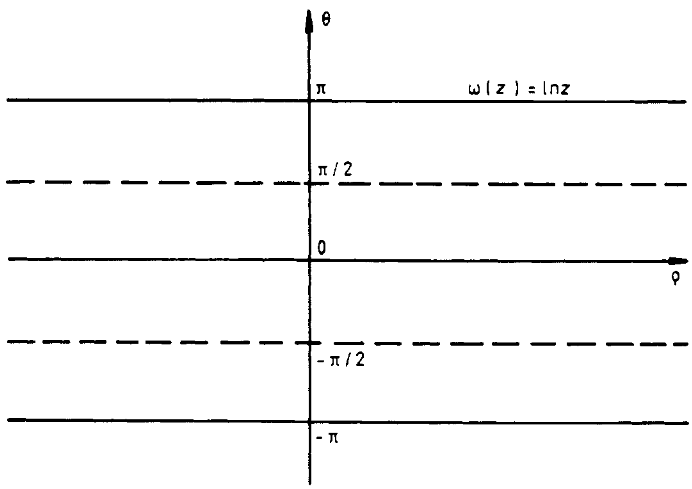

Figure 2. The conformal transformation $\omega = \ln z$ maps the entire plane with a defect line onto a strip with periodic boundary conditions and two equidistant defects.

behaviour of the scaling function near the defect is dominated by the defect exponent η^* (Cardy 1984b) which guarantees the success of the amplitude method in obtaining the defect exponent. It is worthwhile mentioning, however, that the anomalous behaviour of η^* is not shared by x_ε (half the critical exponent of the energy–energy correlation function). To confirm the above statement we write the scaling relation satisfied by the defect free energy f^* (difference between the free energy for the system with defect and the free energy for the homogeneous system) per spin as

$$f^*(t, h, D, h_1) = b^{-1} f^*(b^{y_t} t, b^{y_h} h, b^{y^*} D, b^{y_h^*} h_1) \tag{5}$$

where $t = (T - T_c)/T_c$, h is the bulk magnetic field, h_1 is the magnetic field acting on the defect spins and D is the enhancement of the coupling $(J' - J)/J$. From equations (1) and (5) it follows that D is responsible for the continuous variation of η^*, its scaling dimension y^* being zero, unless J' of figure 1(b) vanishes (in this case $y^* = -1$ as shown by Cardy (1984b)). The anomalous dimension x_ε^* of the energy operator conjugated to the enhanced coupling D is then given by

$$x_\varepsilon^* = 1 - y^* = \begin{cases} 1 & \forall J_1, \forall J_2 \neq 0 \qquad (6a) \\ 2 & \text{if } J_2 = 0. \qquad (6b) \end{cases}$$

Therefore the vanishing of y^* opens the possibility of obtaining non-universal behaviour of η^* but at the same time requires universality of the anomalous dimension of the energy operator ($x_\varepsilon = 2 - 1/\nu$ of the homogeneous Ising model is also equal to 1, since $\nu = 1$). This invariance of x_ε allows us to use conformal invariance methods to investigate non-universality in the Hamiltonian context, where the universal quantities are the ratios of mass gaps (Penson and Kolb 1984, Alcaraz *et al* 1985).

We have studied the Hamiltonians

$$H_1 = -K \sum_{i \neq 1} \sigma_i^z - K_1 \sigma_1^z - K \sum_i \sigma_i^x \sigma_{i+1}^x \tag{7a}$$

and

$$H_2 = -K \sum_i \sigma_i^z - K \sum_{i \neq 1} \sigma_i^x \sigma_{i+1}^x - K_2 \sigma_1^x \sigma_2^x \tag{7b}$$

which correspond to highly anisotropic versions of 2D Ising models with linear defects (see figure 1). In equations (7a) and (7b) σ^x, σ^z are the Pauli matrices. The autocorrelation function of the spin at the defect has a power law decay whose index is

$$\eta_H^* = \left(\frac{2}{\pi} \tan^{-1} \Lambda\right)^2 \tag{8}$$

where

$$\Lambda = K_1/K \tag{9a}$$

for H_1, and

$$\Lambda = K/K_2 \tag{9b}$$

for H_2. These results were derived by Peschel and Schotte (1984) using bosonisation methods but can also be found by taking the Hamiltonian limit in equations (2) and (3). This problem has also been investigated by a real space renormalisation group method (Uzelac *et al* 1981) which does not describe correctly the dependence of η_H^* on Λ.

In this letter we will use the method of the amplitudes which consists in calculating the critical indices through the ratio of the mass gaps of finite rings. To study the defect exponent η_H^* we need to obtain the ground and lowest excited states of the Hamiltonian H_1^N (H_2^N) for finite chains with two defects (at $i = 1$ and $N/2 + 1$) and periodic boundary conditions. Following Lieb *et al* (1981) we perform a Jordan–Wigner transformation (1928) so that H_1^N is given by

$$H_1^N = -2\Big(K_1(c_1^+c_1-\tfrac{1}{2}) + K_1(c_{N/2+1}^+c_{N/2+1}-\tfrac{1}{2}) + \sum_i{}' K(c_i^+c_i-\tfrac{1}{2}) + \sum_i \tfrac{1}{2}K(c_i^+-c_i)(c_{i+1}^+ + c_{i+1}) - \tfrac{1}{2}K(c_N^+-c_N)(c_1^++c_1)[\exp(\mathrm{i}\pi M)+1]\Big) \tag{10}$$

where in (Σ'_i) i takes all values except $i=1$ and $N/2+1$. The fermion creation and annihilation operators c^+, c are given by

$$c_j^+ = \tfrac{1}{2}(\sigma_j^x + \mathrm{i}\sigma_j^y)\prod_{k<j}[-\sigma_k^z] \tag{11a}$$

$$c_j = \tfrac{1}{2}\prod_{k<j}[-\sigma_k^z](\sigma_j^x - \mathrm{i}\sigma_j^y) \tag{11b}$$

$M=\Sigma_j c_j^+c_j$ is the number of fermions, and the parity $p=\mathrm{e}^{\mathrm{i}\pi M}$ is conserved. The Hamiltonian (10), which can be written as

$$H_1^N = -\sum_{i,j}[c_i^+A_{ij}c_j + (c_i^+B_{ij}c_j^+ + \textsc{hc})] \tag{12}$$

with A and B given by†

$$A = 2\begin{pmatrix} K_1 & K/2 & 0 & & & & & \pm K/2 \\ K/2 & K & K/2 & 0 & & & & \\ 0 & K/2 & K & K/2 & & & & \\ & \ddots & \ddots & \ddots & & & & \\ & & & & K/2 & K_1 & K/2 & \\ & & & & \ddots & \ddots & \ddots & \\ \pm K/2 & & & & & & & K \end{pmatrix} \tag{13}$$

and

$$B = 2\begin{pmatrix} 0 & K/2 & & & & \mp K/2 \\ -K/2 & 0 & K/2 & & 0 & \\ & \cdot & \vdots & \vdots & \vdots & \cdot \\ & 0 & & -K/2 & 0 & K/2 \\ \pm K/2 & & & & -K/2 & 0 \end{pmatrix}, \tag{14}$$

can be diagonalised by a new set of quasiparticle (fermion) operators η_α, η_α^+ where

$$\eta_\alpha = \sum_i (g_i^\alpha c_i + h_i^\alpha c_i^+) \tag{15}$$

satisfies the relation (Lieb *et al* 1961)

$$[\eta_\alpha, H_1^N] = \Lambda_\alpha \eta_\alpha \tag{16}$$

with

$$H_1^N = \sum_\alpha \Lambda_\alpha \eta_\alpha^+\eta_\alpha + \text{constant}. \tag{17}$$

† The sign of K in the matrices A and B is fixed by parity.

Substitution of equations (12) and (15) in equation (16) furnishes a system of coupled equations for g^α and h^α which can be written in a more convenient form in terms of the symmetric (ϕ_i^α) and antisymmetric (ψ_i^α) linear combinations of g_i^α and h_i^α. Then we finally get

$$\phi^\alpha(A-B)(A+B)=\Lambda_\alpha^2\phi^\alpha \tag{18a}$$

$$\psi^\alpha(A+B)(A-B)=\Lambda_\alpha^2\psi^\alpha \tag{18b}$$

which allows us to find the 'one-fermion' energies Λ_α by diagonalisation of the matrix $(A+B)(A-B)$. From the invariance of $\mathrm{Tr}[H]$, we obtain the constant in equation (17):

$$\text{constant}=-\tfrac{1}{2}\sum_\alpha \Lambda_\alpha. \tag{19}$$

Proceeding in this way it is possible to obtain exactly the complete spectrum of H_1^N (as well as of H_2^N) for $N\simeq 100$ sites in just 80 s on a VAX 11/780. For comparison we have applied Lanczos' method to find the ground and lowest excited states of those Hamiltonians and for $N=14$ we spent about 20 min on the same computer (this relatively long time is due to the lack of cyclic invariance of the basis states).

Once we have obtained the eigenvalues of H_1^N and H_2^N we get the estimates for η_H^* dividing the first gap:

$$G=E_0^{\text{odd}}-E_0^{\text{even}} \tag{20}$$

where E_0^{odd} (E_0^{even}) is the lowest energy of the odd (even) sector by

$$\tilde{G}=E_1^{\text{even}}-E_0^{\text{even}} \tag{21}$$

where E_1^{even} is the first excited state of the even sector. According to previous papers (Penson and Kolb 1984, Alcaraz *et al* 1985) the ratio $G/\tilde{G}$ is equal to the ratio $(x_\sigma^*/x_\varepsilon^*)$ of the anomalous dimensions of the spin and energy density at the defect. Thus

$$\frac{G}{\tilde{G}}=\frac{x_\sigma^*}{x_\varepsilon^*}=\frac{\eta_H^*}{2x_\varepsilon^*} \tag{22}$$

and according to equation (6*a*) η_H^* is twice the ratio of gaps if $K_2\neq 0$. Our results, shown in tables 1 and 2, are in complete agreement with equation (8) for any value

Table 1. Estimates of the critical index $\eta_{H_1}^*$ obtained by combining finite-size scaling and conformal invariance.

	Λ			
Lattice	0.25	0.50	1.50	3.00
10	0.024 62	0.087 96	0.393 79	0.636 23
20	0.024 40	0.087 34	0.392 03	0.633 20
30	0.024 36	0.087 22	0.391 71	0.632 69
40	0.024 34	0.087 17	0.391 60	0.632 51
50	0.024 33	0.087 16	0.391 55	0.632 43
60	0.024 33	0.087 15	0.391 52	0.632 38
70	0.024 32	0.087 14	0.391 50	0.632 36
80	0.024 32	0.087 13	0.391 49	0.632 34
Exact	0.024 32	0.087 12	0.391 45	0.632 29

Table 2. Estimates of the critical index $\eta^*_{H_2}$ obtained by combining finite-size scaling and conformal invariance.

	Λ			
Lattice	0.25	0.50	1.75	2.50
10	0.715 32	0.499 54	0.110 28	0.059 45
20	0.713 18	0.497 49	0.109 48	0.058 86
30	0.712 76	0.497 10	0.109 34	0.058 75
40	0.712 60	0.496 96	0.109 22	0.058 72
50	0.712 53	0.496 90	0.109 27	0.058 70
60	0.712 49	0.496 86	0.109 25	0.058 69
70	0.712 47	0.496 84	0.109 25	0.058 69
80	0.712 45	0.496 85	0.109 24	0.058 69
Exact	0.712 40	0.496 78	0.109 22	0.058 67

of Λ. We also notice the reasonable agreement already achieved with $N = 10$ (when Lanczos' method is still quick enough).

In conclusion we have used conformal invariance and finite-size scaling to obtain with precision the non-universal index η^*_H of the time correlation function of the spin in defected transverse Ising chains. Extension of this work to other models such as the spin-$\frac{1}{2}$ XY chain as well as a complete study of the corrections to scaling are in progress.

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