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On the validity of the gap-exponent relation in Ising models with many defect lines

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Abstract. Numerical evidence is presented to support the conjecture that the gap-exponent relation remains valid for multi-defect Ising systems where exact solutions are unavailable. Predictions for exponents corresponding to arbitrary lattice anisotropy are given.

1. Introduction

Defect lines represent marginal perturbations to the critical Ising model in two dimensions. Exponents characterising the correlators defined along the defects are expected to vary continuously with the defect strengths (Bariev 1979, McCoy and Perk 1980). The presence of these lines breaks (at least partially) the conformal symmetry. Therefore, the validity of the gap-exponent relation (Luck 1982, Cardy 1984), which connects the anomalous dimensions with the spectrum of the transfer matrix of a finite-width strip is questionable (Turban 1985, Guimarães and Drugowich de Felicio 1986).

This relation has been shown to stay valid in the case when a straight line defect divides the plane into two halves (Peschel and Schotte 1984, Henkel and Patkós 1987b). These authors have solved the spectrum of the Hamiltonian of the strip and compared the levels with the Hamiltonian limit of the exponents derived in the plane with finite anisotropy of the couplings J_x and J_y. Since the continuously varying exponents are not universal (i.e. depend explicitly on the defect strength), it is essential to compare quantities which are calculated using the same kind of regularisation in each geometry connected by the conformal logarithmic map.

Recently, the algebraic interpretation (Baake *et al* 1989) of the exact solution of the strip Hamiltonian with arbitrary, but finite, number of defects (Henkel *et al* 1989) has revealed non-Abelian Kac-Moody-Virasoro algebras generating the spectrum of these systems. In particular, appendix B of Henkel *et al* (1989) contains the conjecture that the generators of this algebra are connected with a subset of conformal Virasoro generators in the plane with a star-like defect configuration (all rays originate from one point in the plane). If this conjecture is correct, then spectrum levels are connected with the exponents of certain, specifically chosen, correlators evaluated with the background of the star-like defect.

One meets two obstacles in verifying the above conjecture. First, to our knowledge there is no analytic or other type of information available for correlators in such multi-defect systems. Second, there is no way to define a time-continuum (Hamiltonian) limit along any one of the defect lines. These questions make difficult any attempt to compare results derived in the strip with data for the above system living on the infinite plane.

In this paper we investigate the gap-exponent relationship for one of the simplest non-trivial many-defect configurations (figure 1(a)), where the defect lines are chosen along the x and y axes.

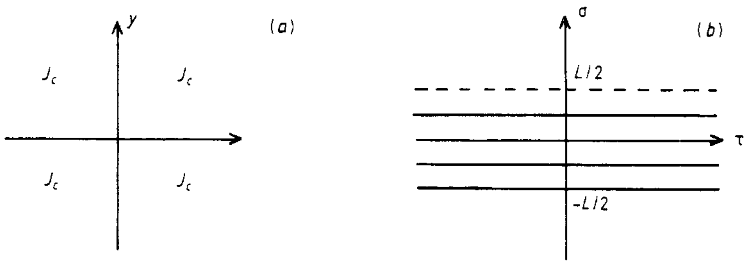

Figure 1. Defect lines in (a) planar geometry and (b) strip geometry.

This choice best fits the square (quadratic) lattice and so minimises the finite-size effects. The possibility of investigating more complicated defect structures is discussed later. Obviously, the present test can provide evidence for the above conjecture but cannot provide a proof. First we shall discuss the choice of the correlation function best suited for the proposed test. Also, we present the spectrum of the strip transfer matrix for arbitrary, finite anisotropy ($J_\sigma \neq J_\tau$) starting from the Hamiltonian expressions of Henkel *et al* (1989). We carefully describe the analysis of the Monte Carlo simulations performed with two different realisations of the defects, namely with both 'line'-type and 'ladder'-type lattice realisations. The exponents in each case are compared, for various values of the defect strength, with predictions from the gap-exponent relation. They provide good evidence for the validity of a conformal connection between the physics of the strip and plane geometries.

2. Correlation functions and lattice regularisation

Consider figure 1(b). The four equidistant defects with equal strengths certainly break translational invariance along the periodic σ-extension of the strip. The lowest excitation in the $Q=1$ (spin) sector of the strip transfer matrix will dominate the behaviour of spin-spin correlations when the τ distance between spins is large. In order to avoid contributions from eigenvalues with non-zero wavenumber, it is convenient to form linear combinations from the spin variables which do respect the discrete remnant of the translational symmetry:

$$C(\tau)_{\text{strip}} = \langle S(\tau=-T)S(\tau=T)\rangle \qquad S(\tau) = \frac{1}{4}\sum_{i=-2}^{1} s\left(\tau, \sigma = \frac{i}{4}L\right). \tag{1}$$

If the logarithmic connection between the strip and the plane works correctly, the correlation function (1) is mapped onto that appearing in figure 2(a).

There are two forms of lattice regularisation for the defects. One may either form 'line' defects, where couplings between the sites on the x and y axes are shifted away from criticality, or one may use a one-site-wide 'ladder' of non-critical couplings to represent each defect line. In the latter case, it is more convenient to measure correlations between the operator configurations appearing in figure 2(b) where each factor is the average of eight spin variables. The aim is to measure the $C(r)_{\text{plane}}$ correlators on symmetric lattices ($J_x = J_y = J_c = 0.440\,687\ldots$), with $J(\text{defect}) = \kappa_{\text{E}} J_c$ for each defected coupling. Particularly in the case of the ladder defect model, the effect of the logarithmic map (from strip to plane) on the correlators is not certain. For example, there will be additional finite-distance effects associated with the proximity of the spin operators to the special point where the defects intersect, further complicated in the ladder case by the finite width of the rungs themselves.

As emphasised above, one can test the gap-exponent relationship only when the same regularisation is applied in each geometry. Hence, one also has to work with 'Euclidean' regularisation in the strip. Starting from the Hamiltonian results of Henkel *et al* (1989) ($J_\sigma \to 0$, $J_\tau \to \infty$) we shall present the expression for the spectrum of the logarithm of the transfer operator for arbitrary finite anisotropy ($J_\sigma \neq J_\tau$). The predictions for the symmetric lattice, in particular, will be compared with the exponent data from Monte Carlo simulations of (1) to be presented below.

The partition function of the most general nearest-neighbour Ising model characterised by the set of couplings $\{J_\sigma(\boldsymbol{x}), J_\tau(\boldsymbol{x})\}$ can be written as

$$Z = \sum_{\{s\}} \prod_{\boldsymbol{x}} \left((1+\tanh J_\sigma(\boldsymbol{x}) s(\boldsymbol{x}) s(\boldsymbol{x}+\hat{\sigma})) \frac{1+\tanh J_\tau(\boldsymbol{x}) s(\boldsymbol{x}) s(\boldsymbol{x}+\hat{\tau})}{1+\tanh J_\tau(\boldsymbol{x})} \right). \tag{2}$$

In (2), after rescaling each factor by an appropriate field-independent expression, one recognises the usual $\exp(J s \cdot s)$ Boltzmann factors. The matrix element of the transfer operator corresponding to (2), in the spin basis $|\{s\}\rangle$, is given as

$$\begin{aligned}\langle\{s'\}|\hat{T}_{x,x+\hat{\tau}}|\{s\}\rangle &= \langle\{s'\}| \prod_l (1+\tanh J_\sigma(l\hat{\sigma}+\hat{\tau})\sigma_l^z\sigma_{l+1}^z)|\{s'\}\rangle \\ &\quad\times\left(1+\sum_k \exp(-2J_\tau(k\hat{\sigma}))\langle\{s'\}|\sigma_k^x|\{s\}\rangle\right. \\ &\quad\left.+\sum_{k\neq l} \exp[-2(J_\tau(k\hat{\sigma})+J_\tau(l\hat{\sigma}))]\langle\{s'\}|\sigma_k^x\sigma_l^x|\{s\}\rangle+\ldots\right)\end{aligned} \tag{3}$$

where σ^x and σ^z are Pauli matrices (to be distinguished from $\hat{\sigma}$ and $\hat{\tau}$ the lattice unit vectors). The omitted terms in the bracket [...] correspond to three or more flips when passing from the configuration $\{s\}$ to $\{s'\}$. The *exact* representation (3) implies that the eigenvalues of $\hat{T}$ depend only on the set of variables $\{\tanh J_\sigma(\boldsymbol{x}), \exp(-2J_\tau(\boldsymbol{x}))\}$.

The Hamiltonian limit is defined following Fradkin and Susskind (1978) by setting

$$\tanh J_\sigma(\boldsymbol{x}) = \kappa_{\text{H}}^{(\sigma)}(\boldsymbol{x}) \tanh J_\sigma \qquad \exp(-2J_\tau(\boldsymbol{x})) = \kappa_{\text{H}}^{(\tau)}(\boldsymbol{x}) \exp(-2J_\tau) \tag{4}$$

with the homogeneous scaling factors $\tanh J_\sigma$ and $\exp(-2J_\tau)$, which obey the relation

$$\lambda \tanh J_\sigma = \exp(-2J_\tau). \tag{5}$$

Choosing

$$J_\sigma \to 0 \qquad J_\tau \to \infty \qquad \lambda \text{ fixed} \tag{6}$$

and for the temporal lattice spacing

$$a_\tau = \tanh J_\sigma \tag{7}$$

one arrives at the Hamiltonian operator of the time-continuum limit

$$\hat{H} = -\sum_l \kappa_{\mathrm{H}}^{(\sigma)}(l)\sigma_l^z\sigma_{l+1}^z - \lambda \sum_l \kappa_{\mathrm{H}}^{(\tau)}(l)\sigma_l^x. \tag{8}$$

The critical Hamiltonian with defects is reached when $\lambda = 1$ and only a finite number of the defect strengths $\{\kappa_{\mathrm{H}}^{(\sigma)}, \kappa_{\mathrm{H}}^{(\tau)}\}$ are different from unity. $\kappa_{\mathrm{H}}^{(\sigma)}$ corresponds to ladder-type and $\kappa_{\mathrm{H}}^{(\tau)}$ to line-type defects. The eigenvalues of the Hamiltonian depend on the defect strengths.

The important observation is that, for the Ising model, one is able to reconstruct from (8), using relations (4) and (7), the most general transfer matrix. The higher flip terms of (3) are completely determined by the information in (8). Therefore, by replacing the κ_{H} dependence of the eigenvalues of (8) by the relations (4) at $\lambda = 1$, we find the critical spectrum for finite anisotropy too. This point can be explicitly illustrated by the following example.

(i) Substituting the bulk Hamiltonian critical point $\lambda = 1$ into (5), one finds the exact condition for criticality in the homogeneous system ($\kappa_{\mathrm{H}}^{(\sigma)} = \kappa_{\mathrm{H}}^{(\tau)} = 1$) for arbitrary finite anisotropy ($J_\tau \neq J_\sigma$).

(ii) In the case of a single defect (either $\kappa_{\mathrm{H}}^{(\sigma)}(l_d) \neq 1$ or $\kappa_{\mathrm{H}}^{(\tau)}(l_d) \neq 1$ on the defect bonds l_d) Peschel and Schotte first found the η exponent for spin-spin correlations in the Hamiltonian limit (Peschel and Schotte 1984). They also observed that, by the replacement (4), the general results of Bariev (1979) and of McCoy and Perk (1980) are recovered.

The above arguments allow us to write down the generalisation to finite anisotropy of the Hamiltonian result of Henkel *et al* (1989) for four equidistant defects of equal strength. The exponents at some value of κ_{H} are given in (2.11) of this paper. We note that, at least for up to four defects, the Hamiltonian spectrum is *identical* for the line and ladder defect models. We have verified this by repeating, for the line defect, the exact solution of the ladder case presented by Henkel *et al.* For the case of four defects, the dominant exponent in the ($Q = 1$) spin sector is given as a function of κ_{H} by (cf equations (2.11), (1.5), (2.17) and (2.18) of Henkel *et al* (1989))

$$x = \{\Delta_1^2 + \Delta_2^2 - 2\Delta_0^2\} - 2\Delta_1 + 1 \tag{9}$$

where the Δ_i are given by

$$\begin{aligned} &\Delta_i = \frac{1}{2} - \frac{\alpha_i}{4\pi} \qquad \alpha_0 = 2\cos^{-1}\left[-\left(\frac{1-\kappa_{\mathrm{H}}^2}{1+\kappa_{\mathrm{H}}^2}\right)^2\right] \\ &\alpha_1 = 2\cos^{-1}\left(-\frac{(\kappa_{\mathrm{H}}^2 + 2\kappa_H - 1)(\kappa_{\mathrm{H}}^2 - 2\kappa_{\mathrm{H}} - 1)}{(1+\kappa_{\mathrm{H}}^2)^2}\right) \qquad \alpha_2 = 2\pi \end{aligned} \tag{10}$$

(Note that, in this normalisation, $x_{\mathrm{Ising}} = \frac{1}{8}$). The exponents at arbitrary anisotropy $\{J_\sigma, J_\tau\}$ are then given by (9), (10) with the Hamiltonian defect strengths $\kappa_H^{(\sigma)}$, $\kappa_{\mathrm{H}}^{(\tau)}$ being replaced by functions of the 'Euclidean' quantities $\kappa_{\mathrm{E}}^{(\sigma)}$, $\sigma_{\mathrm{E}}^{(\tau)}$ as implied by (4), i.e.

$$\kappa_{\mathrm{H}}^{(\sigma)} = \frac{\tanh(\kappa_E^{(\sigma)} J_\sigma)}{\tanh J_\sigma} \qquad \text{ladder} \tag{11}$$

$$\kappa_{\mathrm{H}}^{(\tau)} = \frac{\exp(-2\kappa_E^{(\tau)} J_\tau)}{\exp(-2J_\tau)} \qquad \text{line.} \tag{12}$$

3. Numerical procedures and results

We performed substantial simulations of the critical Ising model with the star-shaped line and ladder defects described above. A sequence of finite $L \times L$ lattices ($L = 8$, 16, 24, 32, 48) with periodic boundary conditions was used and sample defect strengths $\kappa_E = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ and 1 (homogeneous Ising) investigated. The simulation method was based on the spin-coded Metropolis algorithm of Bhanot *et al* (1986) but with an improved stochastic decision list structure (Michael 1986). The idea is that update acceptance decisions are made with the correct probabilities $\exp(J\Delta\mathscr{H})$ by drawing bit patterns randomly from large lists containing carefully chosen multiplicities of each pattern and comparing with the bit representation of the integer $\Delta\mathscr{H}$. Since these multiplicities and the total list population are obviously integers, the probabilities which can be represented (as ratios of these integers) are discretised. In turn, this means that the couplings at which simulations can take place are discretised. The longer the decision list, the more closely can one approach a desired coupling value using an optimal choice of pattern multiplicities. The algorithm was further enhanced to deal with a spin Hamiltonian involving multiple coupling. In this case, the Metropolis update acceptance probability is a function of

$$J\Delta\mathscr{H} = J\Delta\mathscr{H}_h + \kappa J\Delta\mathscr{H}_d \tag{13}$$

and so extra stochastic decision lists are required to deal with updates affecting the homogeneous (h) and defected (d) bond contributions to the change in the total spin Hamiltonian. For the line (ladder) defect case a total of three (five) separate decision lists are required. As in the basic algorithm, the couplings J and κ at which simulations may be performed are discretised. The choice of these is as indicated in table 1. Typical update speeds of 10^6 spins per second were achieved on serial processors of modest power for defected and undefected models alike.

Correlation measurements $C(r)$ and effective exponents defined by

$$x_{\text{eff}}(r) = \frac{1}{2}\,\frac{\log[C(r-1)/C(r)]}{\log[r/(r-1)]} \tag{14}$$

were made only after every so many (N_{decorr}) sweeps in order to decorrelate the measurements in computer time. Variances were calculated from the 32 (=number of bits/word) independent lattices simulated in parallel. Tests were made to determine the optimal value of N_{decorr} which showed correct scaling of the variances with sample

Table 1. Comparison of predicted (see equations (9)-(11)) and measured exponents for line and ladder defect models.

Defect type	κ_E	Predicted	Measured
none	1.0	0.125	0.125 ± 0.001
line	0.749 469	0.206 987	0.203 ± 0.003
line	0.499 186	0.305 695	0.308 ± 0.016
line	0.249 464	0.408 932	0.43 ± 0.07
ladder	0.766 383	0.226 252	0.226 ± 0.012
ladder	0.520 779	0.404 725	0.40 ± 0.05
ladder	0.262 274	0.674 628	0.52 ± 0.10

size but which minimised the relatively expensive ratio of measurement to update time. Most of the data was obtained with $N_{\text{decorr}} = 200$ and involved typically 10^{11} spin updates on each lattice size and at each set of couplings. For computational efficiency, the update algorithm was coded entirely in Boolean operations and was such that the pure Ising limit was achieved in a non-trivial way. This allowed a stringent test of the code in both line and ladder defect cases.

Assuming a single dominant exponent (9), one expects the correlation behaviour at large separation r to be

$$C(r) \sim r^{-2x}. \tag{15}$$

and $x_{\text{eff}}(r)$ to be asymptotically constant $(=x)$. All correlations and exponents, however, showed appreciable finite size effects; at fixed L, $x_{\text{eff}}(r)$ was approximately constant only within some range of r (which, however, increased with L). At fixed r, the effective exponent increased smoothly with L, so offering the possibility of a finite-size extrapolation. This was achieved using the methods of Beleznay (1986) which allow one, in principle at least, to estimate both the convergence exponent and the error on the final extrapolated value. Using high statistics homogeneous Ising model correlation data for lattices of size $L = 8$–48, we found a convergence exponent $\alpha \sim -1$. For the strongly defected lattices, the effective convergence exponent was closer to $-\frac{1}{2}$. The errors quoted below include the uncertainty due to the extrapolation method†. Operator separations (r) between 2 and 4 were used to obtain the data presented and separations up to 6 to check the approximate constancy of the extrapolated exponents x. Although the noise in the larger-r data reduced its value, the consistency of the data provided some evidence that a single exponent dominates this choice of correlator, at least in the line-defect model.

The choice of site for the inner operators (see figure 2(a)) was determined by two observed effects. For a fixed separation r, the relative error on the exponent $x_{\text{eff}}(r)$ (equation (14)) decreased as the inner operators (circles in figure 2) moved closer to the defect intersection. For example, at $r = 3$ on a 24×24 lattice with a line defect of strength $\kappa = 0.749$, the relative error was twice as large when inner operators were three lattice units away from the defect intersection as compared with operators on the intersection itself. This last choice corresponds to the point $\tau = -\infty$ in the strip geometry. The second effect was that finite-size effects were considerably more severe

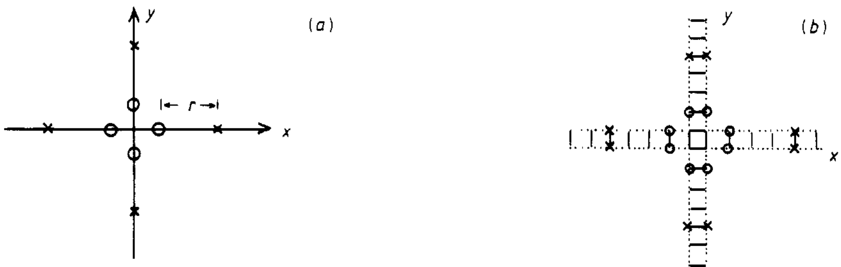

Figure 2. Correlation measurements in planar geometry for (a) line defects and (b) ladder defects. Open circles (crosses) are the images of those forming the operator $S(\tau = -T)$ ($S(\tau = T)$) and r is the operator separation in lattice units.

† Cardy has predicted (Cardy 1986a, 1986b) an asymptotically logarithmic finite-size correction. At the values of L explored (generally up to 32), the finite-size corrections measured appear stronger than this.

for less-central choices of inner operator. The bulk of the data was therefore obtained with the most symmetric and central choice. After finite-size extrapolation, the other choices lead to exponent values which were compatible within the somewhat larger errors. A similar effect was observed with the ladder defect model. The most reliable numerical results were obtained by using operators (see figure 2(*b*)) corresponding to the pairs of spins on each end of a ladder 'rung'. The final results are displayed in table 1.

4. Discussion and conclusions

The predicted and measured spin exponents for the symmetric lattice are in good agreement for the homogeneous Ising model itself and for its variant containing four line defects. When the defects are strong ($\kappa < \frac{1}{2}$), and in particular for the ladder defect model, the poorer accuracy of the data obscures the comparison. A thoroughly reliable test in the ladder case probably requires the distance of the inner spins from the crossing square to be much larger than the width of the ladder itself. The size of lattices and the statistics realistically accessible for this study did not permit us to fulfil this condition. However, at least for moderate defect strengths, the comparison provides evidence that the gap-exponent relation is satisfied for both models of the defects.

Access to larger lattices would also allow tests of more complicated defect structures with non-rectangular intersections and/or multiplicities greater than four. In the continuum limit, the step-wise representation of such defects on a quadratic lattice should be adequate and the finite-size effects kept sufficiently under control. In this way we would expect to verify the gap-exponent relation for defect angles which are arbitrary but subject to the commensurability condition of Henkel *et al* (1989).

The present successful comparison completes the analysis of defected Ising systems in terms of Kac-Moody-Virasoro algebras initiated by Henkel and Patkos (1987a, 1987b) and developed by Henkel *et al* (1989) and Baake *et al* (1989). Although conclusive proof is still lacking, it does represent a non-trivial positive argument that the generators of the Hamiltonian spectrum of the strip are connected with a subset of the conformal generators in the plane even in the presence of multiple defects.

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