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INVESTIGATION OF THE 3-STATE, 2-D POTTS MODEL
WITH ONE DEFECT LINE OF COUPLINGS BY DENSITY
OF STATES MONTE CARLO METHOD

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Abstract

The critical 3-state two-dimensional Potts model with one line of defect couplings has been studied. Interpolating the coupling strength between the free and periodic boundary conditions renormalization group arguments suggest that the algebraic content should change discontinuously. Monte Carlo data on different sized and shaped lattice systems have been collected. Predictions for the surface-free energy density, the central charge and the magnetization two-point correlation scaling dimension are given. The results appear to contradict to the first order renormalization group expectations.

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1. INTRODUCTION

For two-dimensional systems, conformal invariance plays a central role in a detailed description of the critical point. This allows in particular the identification of the complete operator content of a given model (that is, to obtain the scaling dimensions of all relevant marginal and irrelevant operators). This permits, for example, the exact calculation of the partition function or n -point correlation functions (for reviews see refs [1] and [2]). Minimal theory models with $c < 1$, such as the Ising and the Potts, can be solved exactly because the number of primary operators of the Virasoro algebra is finite and the partition functions can be explicitly constructed [3].

Defect lines — along which the coupling is different from the bulk — partially break the conformal symmetry, thereby changing the underlying algebra. Recently, Baake et al. [4] gave the algebraic interpretation to the exact solution (Henkel et al. [5]) of the Ising strip Hamiltonian with arbitrary, but finite number of defects. For $n > 2$ -state Potts models no such exact conclusion has been reached because this model cannot be converted into a free fermionic representation, and the Bethe ansatz solution is not appropriate for the periodic-free interpolation.

Bray and Moore [6] have shown that the crossover exponent, governing the stability of the fixed point of the periodic system is given by $\Phi^B = 1 - \nu$, where ν is the correlation length critical exponent, which is connected to the scaling dimension by $\nu = \frac{1}{2-x_\epsilon}$. Thus, the bulk fixed point is stable, unstable and marginal with respect to the defect line perturbation for $\nu > 1$, $\nu < 1$, $\nu = 1$, respectively.

On the other hand, the stability of the fixed point of a system with free boundary condition depends on the crossover exponent Φ^0 , which according to Burkhardt and Eisenriegler [7] is given by $\Phi^0 = 2 - \alpha - \nu - 2\beta_1^0$, where α is the specific heat exponent and β_1^0 is the surface magnetization exponent.

For the Ising model $\Phi^B = 0$, $\Phi^0 = 0$, thus the fixed points are marginal in accordance with the continuous change of the algebra (Henkel et al. [5]). However, for the 3-state Potts model $\Phi^B = 1/6$, $\Phi^0 = -5/18$ (calculating β_1^0 from $\epsilon = d - 6$ expansion one gets $\Phi^0 = 39/6$); and one expect the renormalization flow to start from the instable $\kappa = 1$ bulk fixed point and to end in the $\kappa = 0$ stable, free surface fixed point.

The different algebraic contents of the 3-state Potts model for periodic and free boundary conditions are known exactly [8]. The above renormalization arguments suggest an abrupt change in the algebra, most probably at $\kappa = 1$ unlike to the Ising model.

The aim of my investigation was to test this expectation by the systematic study of different sized and shaped Euclidean lattices. The finite size scaling study of free energy and the leading conformal terms has been carried out. The convergence to the thermodynamic limit is very slow (Schlottmann [9], much slower than that of the Ising model and one should go further to larger lattice sizes to see the disappearance of the “smoothing out” of the jump. Still one may see a tendency towards a jump at $\kappa = 0$ in the thermodynamic limit.

The method I used is based on the calculation of the partition function of the 2-dimensional rectangular lattices. Finite size effects are unknown and complex functions

of both sizes. This work also sheds some light on the shape dependence of the finite size effects. The results are checked against the exactly known expressions of the partition function for free and periodic conditions, $\kappa = 0(1)$, respectively. The partition function is calculated by the “density of states” Monte Carlo method (Bhanot et al. [10] and Karliner et al. [11]).

2. THE MODEL

The 3-state Potts model on different n by m square lattices, with a defect line of strength κ parallel to the x axis and with its periodic boundary condition along the x direction was investigated

$$H^{nm}(\kappa) = - \sum_{x=1}^{n-1} \sum_{y=1}^m \delta(\sigma_{x,y}, \sigma_{x+1,y}) - \sum_{y=1}^m \kappa \delta(\sigma_{n,y}, \sigma_{1,y}) - \sum_{x=1}^n \sum_{y=1}^m \delta(\sigma_{x,y}, \sigma_{x,y+1}) . \quad (1)$$

I have studied this model by calculating the $Z_{cr}^{nm}(\beta = \beta_{cr} = 1.00505254, \kappa)$ critical partition function interpolating between the exactly solved $\kappa = 1$ periodic and $\kappa = 0$ free boundary systems. The free energy is obtained from the continuum limit model by finite size corrections

$$F^{nm}(\kappa) = f_{bulk}nm + s(\kappa)m + F_{conf}(\kappa) + f.s.corr. , \quad (2)$$

where the non-universal bulk term is known (Wu [12]), and the conformal energy can be obtained for the periodic case

$$F_{conf}(\kappa = 1) = -\frac{\pi c\tau}{6} - \ln \left(\sum_{pq\bar{p}\bar{q}} N_P(p, q, \bar{p}, \bar{q}) \chi_{\bar{p}q}(\tau) \chi_{\bar{p}\bar{q}}(\tau) \right) \quad (3)$$

and for the free boundary case (Cardy [8])

$$F_{conf}(\kappa = 0) = -\frac{\pi c\tau}{24} - \ln \left(\sum_{pq} N_F(p, q) \chi_{pq}(\frac{1}{2}\tau) \right) \quad (4)$$

from the character expansion. Here c is the conformal anomaly number, it is equal to $\frac{4}{5}$ for the 3-state Potts critical model, $\tau = \frac{m}{n}$. The expressions under the logarithm can be calculated with the help of tables of scaling dimensions (Cardy [8]).

Owczarek and Baxter [13] have recently given a formula for the surface-free energy density of the free Potts model by the Bethe ansatz solution

$$s(\kappa = 0) = \ln \left(\frac{\sin(\frac{\pi}{8})}{\sin(\frac{\pi}{24})} \right) - 2 \int_{-\infty}^{\infty} \frac{sh(\frac{\pi}{12}y)sh(\frac{\pi}{3}y)ch(\frac{5\pi}{12}y)ch(\frac{\pi}{12}y)}{ysh(\pi y)ch(\frac{\pi}{6}y)} dy . \quad (5)$$

One can find its value by the numerical integration: 0.5694682288...; these exactly known data will provide the possibility to check the method in sect. 4.

3. THE METHOD

In order to get the value $Z_{cr}^{nm}(\beta)$ I have used the “density of states” method (Bhanot et al. [10]). Several modifications have been compared empirically, i.e. different bandwidths, trial flips, gaussian distribution instead of rigid energy band boundaries, weight function, weighted gaussian, etc.

In each band with the width of b , I started the algorithm from 8–10 independent and different energy configurations in order to provide a check of the ergodicity condition. Having determined the histograms $\{F(E_i^j) \mid 0 \leq i \leq b, 1 \leq j \leq \text{number of sets}\}$, I calculated the ratios of multiplicities, viz.

$$R_i^j = \frac{F(E_i^j)}{F(E_0^j)}. \quad (6)$$

The normalization between subsequent sets can be done at overlapping energies

$$N(E_0^j) = N(E_0^{j-1})R_b^{j-1}, \quad (7)$$

so the midband $0 < i < b - 1$ energies do not increase the error propagation.

This benefit could not be exploited when I used gaussian acceptance distribution instead of rigid band boundaries

$$A(E) = e^{-\frac{(E-E_m)^2}{\sigma^2}}, \quad (8)$$

where E_m is the peak of the curve and σ determines the shape. This acceptance clearly yields a relative occurrence

$$F_g(E) \rightarrow N(E)A(E), \quad (9)$$

from which the estimate of non-normalized $N(E)$ can easily be reconstructed by dividing $A(E)$. This gives the ratios

$$R(E_i) = \frac{F_g(E_i)/A(E_i)}{F_g(E_{i-1})/A(E_{i-1})} \quad (10)$$

within the σ neighbourhood of the E_m well, so the distribution has to be shifted along the whole energy scale in order to collect information for each energy. As a matter of fact, we only need to know the low-energy multiplicities because the exponential cut-off is in the partition function. If we obtain sufficiently good estimates for the desired $R(E_i)$, normalization can be done by subsequent energies

$$N(E_i) = N(E_{i-1})R(E_i). \quad (11)$$

This produces a larger error propagation than in eq. (7). Alternatively, if we choose some arbitrary low E_0 and high E_b say: $E_0 = E_m - \sigma$, $E_b = E_m + \sigma$ and store only the ratios

$$R_i^j = \frac{F_g(E_i)/A(E_i)}{F_g(E_0)/A(E_0)}, \quad 1 \leq i \leq b; \quad (12)$$

following the j -th completed histogram similarly to eq. (6), we lose the information outside this (E_0, E_b) region.

It was necessary to apply the balancing weighting function $s_W(E)$ for bigger volume lattices V . Each link is accepted with probability

$$\min(1, \exp[-V(s_W(E') - s_W(E))]) \quad (13)$$

in the band, or

$$\min(1, A(E)\exp[-V(s_W(E') - s_W(E))]) \quad (14)$$

for the gaussian version, where E' is the new energy and E is the original energy. The justification of this procedure can be found in my Appendix. I concluded that the gaussian version with or without weighting yielded larger errors than the original algorithm and it is recommended only in such cases when ergodicity is not easily satisfied, like for spin glass systems.

The method applied in this study is similar to that of Karliner et al. [11]. In order to determine the weighting function, the algorithm without weighting ($s_W(E) = 0$) was run first with narrow 4 bins per set. The bandwidth of the weighted run was usually 7 bins. A $10^7 - 32 \times 10^7$ flip/band was necessary for different lattice sizes to reduce the statistical error below 1%. Exact multiplicities have been determined for low energies by some combinatorics and then used for the absolute normalization of the results.

One can get the $Z(\kappa)$ function for an arbitrary κ defect strength too, by using the technique first proposed by Ferrenberg et al. [14]. If one divide the energy to the bulk and surface terms

$$E = E_1 + \kappa E_2, \quad (15)$$

$$E_1 = - \sum_{bulk} \delta(\sigma\sigma'), \quad (16)$$

$$E_2 = - \sum_{surf.} \delta(\sigma\sigma'), \quad (17)$$

the $Z(\kappa, \beta)$ function can be easily determined, if the multiplicity of states is known for each E_1, E_2

$$Z(\kappa, \beta) = \sum_{E_1} \sum_{E_2} N(E_1, E_2) e^{-\beta(E_1 + \kappa E_2)}. \quad (18)$$

The ' (prime) index means the nearest neighbour. This enables us to get the whole $Z(\beta, \kappa)$ function from calculating only at one — namely at the $\kappa = 0$ free — coupling strength, and increase the possibility to locate a jump.

Having obtained the total free energy as the logarithm of $Z(\kappa, \beta)$, first I subtracted the exactly known bulk term. The surface-free energy can be calculated from different sized, similarly shaped lattices, since the conformal terms depend only on τ , thus they cancel each other

$$s(\kappa) = \frac{(F^{n_1 m_1}(\kappa) - f_{bulk} n_1 m_1) - (F^{n_2 m_2}(\kappa) - f_{bulk} n_2 m_2)}{m_1 - m_2} + f.s.corr. \quad (19)$$

The next step was to give an estimate for the effective central charge

$$\frac{c}{b(\kappa)}, \quad (20)$$

where $c = 4/5$ and the denominator is a function of κ

$$b(\kappa) = \begin{cases} 6 & \text{for } \kappa = 1, \\ \text{unknown} & \text{for } 0 < \kappa < 1, \\ 24 & \text{for } \kappa = 0. \end{cases}$$

This term can be extracted from $\tau \gg 1$, strip-like systems, since if conformal symmetry holds for $0 < \kappa < 1$, the contributions of conformal operators are exponentially suppressed

$$F_{conf}(\kappa, \tau \gg 1) = \frac{\pi c \tau}{b(\kappa)} + \ln \left(\sum_n e^{-2\pi x_n \tau} \right) \sim \frac{\pi c \tau}{b(\kappa)}, \quad (21)$$

i.e. only the trivial identity $x_0(\kappa) = 0$ term is non-negligible under the logarithm.

The further fit for the lowest $x_1(\kappa)$ scaling dimension can be extracted from intermediate $\kappa = 2.5$ systems following the subtraction of the central charge term (eq. (21)) from $F_{conf}(\kappa, \tau = 2.5)$ and taking the following simplified conformal ansatz

$$\ln \left(\sum_n e^{-2\pi x_n \tau} \right) \sim \ln (e^{-2\pi x_0 \tau} + 2e^{-2\pi x_1 \tau}) \quad (22)$$

omitting the contributions of higher dimension and secondary fields in the sum. The factor 2 in the second term comes from the double degeneracy of the first excited eigenvalue of the $Z(3)$ symmetrical model. The validity of these approximations can be checked by the periodic eq. (3) and free eq. (4) boundary models (tables 1 and 2).

Table 1 Approximations of the exact $F_{conf}(\kappa = 1, \tau)$ of eq. (3) by the leading and the further two lowest eigenvalue terms

τ	2	2.5	8
$F_{conf}(\kappa = 1, \tau)$	1.15583	1.26737	3.35349
$\frac{\pi c \tau}{6}$	0.83775	1.04719	3.35103
$\frac{\pi c \tau}{6} + \ln(e^{-2\pi x_0 \tau} + 2e^{-2\pi x_1 \tau})$	1.15579	1.26736	3.35348

Table 2 Approximations of the exact $F_{conf}(\kappa = 0, \tau)$

τ	2	2.5	8
$F_{conf}(\kappa = 0, \tau)$	0.23938	0.27239	0.83776
$\frac{\pi c \tau}{24}$	0.20943	0.26179	0.83775
$\frac{\pi c \tau}{24} + \ln(e^{-2\pi x_0 \tau} + 2e^{-2\pi x_1 \tau})$	0.23931	0.27238	0.83775

For $\tau = 8$ systems the central charge term (second row) itself reproduces the whole conformal energy, while for $\tau = 2.5$ the additional logarithmic scaling dimension term (eq. (22)) is necessary to get the conformal energy with 10^{-5} accuracy (third row). This observation enables one to calculate the conformal term (eq. (20)) from the measured partition function of $\tau = 8$ lattices and to estimate the lowest, non-trivial x_1 scaling dimension from $\tau = 2.5$ lattices by a further fitting step. These two steps of gradual fitting of the free energy will be exploited in what follows.

4. RESULTS

Estimates for the surface-free energy density (eq. (19)) has been extracted from similar shaped pairs of lattices. The data in table 3 are calculated following the subtraction of the exact bulk term given by eq. (19). The measured values have converging tendency to the exactly known values at $\kappa = 0$ and $\kappa = 1$.

Table 3 The $s(\kappa)$ surface-free energy density scaling for periodic and free boundary conditions

	$8 \times 64 - 32 \times 4$	$8 \times 20 - 6 \times 15$	$10 \times 20 - 6 \times 12$	$6 \times 15 - 4 \times 10$	$6 \times 12 - 5 \times 10$	$5 \times 10 - 4 \times 8$
$s(0)$	-0.568(6)	-0.567(2)	-0.567(1)	-0.571(1)	-0.573(3)	-0.578(2)
$s(1)$	0.0004(2)	0.001(1)	0.001(1)	0.0063(9)	0.003(3)	0.007(1)

Figure 1 shows the $s(\kappa)$ function of these lattices.

The finite size effect is a complex function of both sides so I compared the conformal energies of similar shaped lattices for the exactly known $\kappa = 0$ and $\kappa = 1$ boundary conditions. The exact conformal energies of eqs (3) and (4) can be calculated with the help of known operator content. In figs 2(a) to 2(e) the conformal energy is obtained from the measured free energy following subtraction of the exact bulk and surface energy terms (eq. (5)). Simple linear fitting shows that the scattering and the statistical error of these data are quite good; however, the deviation from the exact value can be a few percent owing to the finite size effect. I have tested the FSS of the conformal energy of $\tau = 2$ systems at an intermediate $\kappa = 0.5$ coupling too (fig. 2(f)). The energy differences are not greater than at the boundaries, so I expect that the results of this paper in the $0 < \kappa < 1$ coupling region have similar magnitude of finite size correction, what can be seen at $\kappa = 0$ and $\kappa = 1$.

Following the line described in sect. 3, in order to get $\frac{c}{b(\kappa)}$ and $x_1(\kappa)$ by two steps of fitting, first I have calculated the effective central charge term from different sized $\tau = 8$ lattices (fig. 3). The surface-free energy function that I used comes from the largest $\tau = 2$ lattices (6×12 to 10×20). The slope of curves at the boundaries and the sequence of different-sized lattices suggest that a jump could occur at $\kappa = 0$ in the $n, m \rightarrow \infty$ limit. Similar conclusion can be drawn if the $s(\kappa)$, which one has to subtract from the free energy, is calculated from other lattice pairs: 4×32 to 8×64 , 6×15 to 8×20 or a combination of them.

Having determined the effective central charge function, I attempted to make an estimate for the lowest non-trivial $x_1(\kappa)$ scaling dimension given by eq. (22) from $\tau = 2.5$ systems. Figure 4 shows these results calculated from 4×10 , 6×15 and 8×20 systems. Observing the boundary slopes and the sequence of these functions, one can again suspect that a jump might occur at $\kappa = 0$. However, the error which comes from the propagation of surface-free energy inaccuracies and finite-size effects is larger too and the estimates for $x_1(0)$, $x_1(1)$ are shifted from the exact values.

I also plotted the results of Schlottmann [9] obtained from numerical diagonalization of the transfer matrix of the one-dimensional $L = 2 - 11$ quantum Potts chains. Since those data are based on the anisotropic regularization; in the Appendix, I worked out

the transformation between symmetrical and anisotropic limits. His results for the primary $x_1(\kappa)$ seem to be in contradiction with mine. However, his secondary $x_1(\kappa)$ scaling dimensions, which are said to be less exactly determined, fit the curves of this paper.

This again emphasizes the fact that larger — perhaps of the order of $m, n \sim 100$ — systems should be investigated to see the disappearance of finite size effects.

5. CONCLUSIONS

The Monte Carlo method based on the determination of the density of states has been applied with success for calculating the partition function of the 2-dimensional 3-state Potts model with one ladder type defect line. Combined with the Ferrenberg-Swendsen type histogramming, numerical estimates for the surface-free energy density, effective central charge and lowest non-trivial scaling dimension as functions of defect strength is given. These functions are derived from bulk physical quantity — $Z_c(\kappa)$ — by gradual fitting. The finite size scaling study confirms the reliability of the applied method and shows that such important physical quantities can be estimated despite of the strong finite size effects. The results appear to support the discontinuity jump of the critical quantities as functions of κ unexpectedly at $\kappa = 0$, contrary to first-order renormalization group expectations. However, they also show the need of further investigation on larger-sized systems.

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INTERPOLATION BETWEEN THE ANISOTROPIC AND SYMMETRIC LIMIT OF THE 3-STATE POTTS MODEL

In this Appendix, I show the connection between the symmetrical Euclidean and the anisotropic Hamiltonian regularization of the 3-state Potts model with arbitrary couplings. Let me denote the horizontal couplings by

$$K_i = K \kappa_E^K(i) \quad (\text{A1})$$

and the vertical ones by

$$L_i = L \kappa_E^L(i) . \quad (\text{A2})$$

The transfer matrix equation can be written as

$$\prod_i \left(1 + (e^{K_i} - 1) \delta(s'_i, s'_{i+1}) \right) \sum_{\{s_i\}} \prod_i \left(1 + (e^{L_i} - 1) \delta(s_i, s'_i) \right) \Psi(s) = \lambda \Psi(s') , \quad (\text{A3})$$

where s_i - s are the spin variables. The equation can be represented in a 3^N -dimensional vector space

$$s_i = 1 \otimes 1 \otimes \dots \otimes s \otimes 1 \dots \otimes 1 , \quad (\text{A4})$$

where the basis states at a single site are

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \quad (\text{A5})$$

The summation for all different horizontal spin chain configurations $\sum_{\{s_i\}}$ can be written as the sum of the “non-flipped” $\{s\} = \{s'\}$ spin chain term, plus terms where one spin is different, plus terms where two spins are different, ... etc. The one-flip part is represented by the matrix

$$\begin{pmatrix} e^{L_i} & 1 & 1 \\ 1 & e^{L_i} & 1 \\ 1 & 1 & e^{L_i} \end{pmatrix} = e^{L_i} \left[1 + e^{-L_i} (\Gamma + \Gamma^\dagger) \right] , \quad (\text{A6})$$

where

$$\Gamma = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} . \quad (\text{A7})$$

In the Hamiltonian limit L is large and the multi-flip actions are negligible, and

$$\prod_i \left(1 + (e^{L_i} - 1) \delta(s_i, s'_{i+1}) \right) \rightarrow \left(\prod_i e^{L_i} \right) \left(1 + \sum_i e^{-L_i} (\Gamma_i + \Gamma_i^\dagger) \right) , \quad (\text{A8})$$

where

$$\Gamma_i = 1 \otimes 1 \otimes \dots \otimes \Gamma \otimes 1 \dots \otimes 1 . \quad (\text{A9})$$

The non-flipped configuration gives also a trivial constant contribution to the $\sum_{\{s_i\}}$ sum

$$\left(\prod_i e^{L_i} \right) . \quad (\text{A10})$$

The diagonal part of the transfer matrix is transcribed in this basis as

$$1 + (e^{K_i} - 1)\delta(s'_i, s'_{i+1}) \rightarrow 1 + \frac{e^{K_i} - 1}{3}(\sigma_i \sigma_{i+1}^\dagger + \sigma_i^\dagger \sigma_{i+1} + 1) , \quad (\text{A11})$$

where

$$\sigma_i = 1 \otimes 1 \otimes \dots \otimes \begin{pmatrix} 1 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega^2 \end{pmatrix} \otimes 1 \dots \otimes 1 \quad (\text{A12})$$

and ω is the cubic root of 1 : $e^{\frac{2\pi i}{3}}$. One easily checks this by considering the followings: if σ_i and σ_{i+1} take the same eigenvalue

$$\frac{e^{K_i} - 1}{3}(\sigma_i \sigma_{i+1}^\dagger + \sigma_i^\dagger \sigma_{i+1} + 1) \rightarrow \frac{e^{K_i} - 1}{3}3 ,$$

if σ_i and σ_{i+1} are different, one can have either

$$\begin{aligned} 1\omega + 1\omega^2 + 1 &= 0 , \\ 1\omega^2 + 1\omega^\dagger + 1 &= 0 , \\ \omega\omega^\dagger + \omega^\dagger\omega^2 + 1 &= 0 . \end{aligned}$$

After rescaling the eigenvalues, the transfer operator looks like

$$\prod_i \left[1 + \frac{e^{K_i} - 1}{3}(\sigma_i \sigma_{i+1}^\dagger + \sigma_i^\dagger \sigma_{i+1} + 1) \right] (1 + \sum_i e^{L_i}(\Gamma_i + \Gamma_i^\dagger)) , \quad (\text{A13})$$

which goes in the limit $K \rightarrow 0$ to

$$1 + \frac{1}{3} \sum_i (e^{K_i} - 1)(\sigma_i \sigma_{i+1}^\dagger + \sigma_i^\dagger \sigma_{i+1} + 1) + \sum_i e^{-L_i}(\Gamma_i + \Gamma_i^\dagger) . \quad (\text{A14})$$

Choosing

$$K \rightarrow 0 \quad L \rightarrow \infty \quad \text{with} \quad \frac{1}{3}(e^K - 1)e^L \sim \frac{1}{3}(e^K - 1)(e^L - 1) = x \quad \text{fixed}, \quad (\text{A15})$$

and for the temporal lattice spacing

$$a_t = -\frac{3\sqrt{3}}{2}e^{-L} , \quad (\text{A16})$$

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

$$H = -\frac{2}{3\sqrt{3}} \left(\sum_i x \kappa_H^K(i)(\sigma_i \sigma_{i+1}^\dagger + \sigma_i^\dagger \sigma_{i+1}) + \sum_i \kappa_H^L(i)(\Gamma_i + \Gamma_i^\dagger) \right) . \quad (\text{A17})$$

The $\frac{3\sqrt{3}}{2}$ factor was chosen to uncover conformal invariance of the Hamiltonian (von Gehlen et. al. [15]). The $x = 1$ gives the correct bulk criticality condition for the isotropic model too

$$K = L = \ln(\sqrt{3} + 1) . \quad (\text{A18})$$

One can transform eq. (A17) with a similarity operation — which exchanges σ_i with $\Gamma_i^\dagger$ — exactly to the usual Hamiltonian form. From eq. (A17) one can see that the Euclidean quantities, which are functions of $\kappa_E^K(i)$ or $\kappa_H^L(i)$ can be transformed to Hamiltonian quantities by

$$\kappa_H^K(i) = \frac{e^{K\kappa_E^K(i)} - 1}{e^K - 1} , \quad (\text{A19})$$

for horizontal defected couplings and

$$\kappa_H^L(i) = \frac{e^{L\kappa_E^L(i)}}{e^L} \quad (\text{A20})$$

for vertical ones similarly to the Ising model [16].

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FIGURE CAPTIONS

- Fig. 1** The surface-free energy density calculated by eq. (19) from 6 pairs of lattices (table 3). Statistical errors are smaller than the deviation of most different curves.
- Fig. 2** (a) – (e) show the finite size scaling of the conformal energy for differently shaped (τ) systems at $\kappa = 0$ and $\kappa = 1$, where the surface-free energy is exactly known. Coefficients of $p2\frac{1}{m} + p1$ linear fitting are also shown. The exact values are: $a = 0.23938$; $b = 1.15583$; $c = 0.27239$; $d = 1.26737$ and $e = 0.33578$.
- (f) is a check of finite size effects in the $\kappa = 0.5$ intermediate region for $\tau = 2$ lattices. The statistical error is greater here since it was calculated with the help of a non-exact surface-free energy. The finite size effects are not greater than for $\kappa = 0$ and $\kappa = 1$ boundary conditions.
- Fig. 3** Effective central charge $c/b(\kappa)$ calculated from 4×32 (solid line), 5×40 (dashed line) and from 8×64 (pointed line) lattices. The surface-free energy used here is obtained from the 6×12 to 10×20 systems. The size of errors are less than the deviation of the curves.
- Fig. 4** The lowest $x_1(\kappa)$ (non-identity) scaling dimension obtained from 4×10 (dashed line), 6×15 (pointed line) and from 8×20 (point-dashed line) free-energy lattice results. Statistical errors are around 10% due to error cumulation. The solid line is the result of Schlottmann; it comes from numerical diagonalization of the transfer matrix of $L = 2 - 11$ Potts quantum chains.

Surface free energy density

Fig. 1

Finite size scaling of conformal energy

Fig. 2

Effective central charge $c/b(\kappa)$

Fig. 3

x_1 scaling dimesion

Fig. 4