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Numerical tests of conjectures of conformal field theory for three-dimensional systems

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Abstract. The concept of conformal field theory provides a general classification of statistical systems on two-dimensional geometries at the point of a continuous phase transition. Considering the finite-size scaling of certain special observables, one thus obtains not only the critical exponents but even the corresponding *amplitudes* of the divergences analytically. A first numerical analysis brought up the question whether analogous results can be obtained for those systems on three-dimensional manifolds.
Using Monte Carlo simulations based on the Wolff single-cluster update algorithm we investigate the scaling properties of $\mathrm{O}(n)$ symmetric classical spin models on a *three-dimensional*, hyper-cylindrical geometry with a toroidal cross-section considering both periodic and antiperiodic boundary conditions. Studying the correlation lengths of the Ising, the XY, and the Heisenberg model, we find strong evidence for a scaling relation analogous to the two-dimensional case, but in contrast here for the systems with *antiperiodic* boundary conditions.

Keywords: Spin models; Finite-size scaling; Universal amplitudes; Conformal field theory

1 Introduction

Statistical mechanical systems at a critical point are essentially characterized by a loss of length scales: as the correlation length diverges, the system becomes a self-similar random fractal. Augmenting this symmetry with translational and rotational invariance in the continuum limit establishes the so-called *conformal* invariance of the system. As the 2D conformal group is of infinite dimension, exploiting this feature allows a complete classification of models of statistical mechanics according to their operator content in two dimensions [1, 2]. This includes a special class of formally model independent relations, like finite-size scaling (FSS) laws; in particular, for the 2D strip geometry $S^1 \times \mathbb{R}$ with periodic boundary conditions Cardy [3] has shown, that for any primary, i.e. conformally covariant, operator of a model showing critical behavior the corresponding correlation length scales as:

$$\xi_i = \frac{A}{x_i} L, \tag{1}$$

where L denotes the circumference of the cylinder, x_i is the scaling dimension of the considered operator, a combination of the classical critical exponents, and $A = 1/2\pi$ in the 2D case.

For 3D systems, however, the situation is different. First, the concept of a primary operator becomes at least problematic (it might possibly be established in terms of the operator product expansion (OPE) [4]). Secondly, numerically feasible and more widely applicable geometries like that of a column $S^1 \times S^1 \times \mathbb{R}$ are not conformally related to flat spaces like in the above mentioned 2D case, which is a essential ingredient of the derivation of relation (1). A transfer matrix calculation by Henkel [5, 6] for the $S = \frac{1}{2}$ Ising model on the column geometry gave for the ratio of the correlation lengths of the magnetization and energy densities the values $\xi_\sigma/\xi_\epsilon = 3.62(7)$ and 2.76(4) for periodic and antiperiodic boundary conditions, respectively. Comparing this with the ratio of scaling dimensions of $x_\epsilon/x_\sigma = 2.7326(16)$ [7] results in the astonishing, theoretically obscure, conjecture that a relation of the form (1) can be re-established in the 3D case, when applying *antiperiodic* (apbc) instead of periodic (pbc) boundary conditions along the torus directions, which later on could be affirmed by a Metropolis Monte Carlo (MC) simulation by Weston [8].
If this result could be established analytically, it would be one of the rare rigorous statements for non-trivial 3D systems. As simulational data were available up to this point only for the single special case of the Ising model, we thought it rewarding to analyze some further models, so possibly establishing this conjecture at an empirical level, which should constitute a motivation and basis for further analytical studies.

2 Models

In generalization to the Ising case we restrict ourselves to the class of O(n) symmetric classical spin models with Hamiltonian

$$\mathcal{H} = -J \sum_{<ij>} \mathbf{s}_i \cdot \mathbf{s}_j, \quad \mathbf{s}_i \in S^{n-1}, \tag{2}$$

assuming nearest-neighbor, ferromagnetic ($J > 0$) interactions. The simulations were done for a discrete sc lattice with dimensions (L_x, L_y, L_z), choosing $L_x = L_y$ and $\xi/L_z \ll 1$, therewith approximately modelling the column geometry $S^1 \times S^1 \times \mathbb{R}$.

3 Simulation and data analysis

The MC simulations were done using the Wolff single-cluster updating scheme [9], as it is known to be more efficient than the Swendsen-Wang [10] update in three dimensions [11]. In order to be able to perform simulations for both, periodic and antiperiodic boundary conditions, the Wolff update had to be adapted to the latter case: this was achieved by exploiting the fact that antiperiodic bc are equivalent to the insertion of a seam of anti-ferromagnetic bonds along the boundary in the case of nearest-neighbor interactions.
To test for a relation according to (1) we had to measure at least two different correlation lengths of the systems under consideration. Following Henkel and in an analogy to the 2D Ising case, where the only non-trivial primary operators are the densities of magnetization and energy, we recorded the correlation functions of these two operators:

$$\begin{aligned} G^c_\sigma(\mathbf{x}_1, \mathbf{x}_2) &= \langle \mathbf{s}(\mathbf{x}_1) \cdot \mathbf{s}(\mathbf{x}_2) \rangle - \langle \mathbf{s} \rangle \langle \mathbf{s} \rangle, \\ G^c_\epsilon(\mathbf{x}_1, \mathbf{x}_2) &= \langle \epsilon(\mathbf{x}_1)\, \epsilon(\mathbf{x}_2) \rangle - \langle \epsilon \rangle \langle \epsilon \rangle. \end{aligned} \tag{3}$$

Variance-reduction of the estimators for these observables can be achieved in a first step by the trivial average over values with $(\mathbf{x}_1 - \mathbf{x}_2) \parallel \hat{e}_z$ and $i \equiv |\mathbf{x}_1 - \mathbf{x}_2| = \text{const}$;

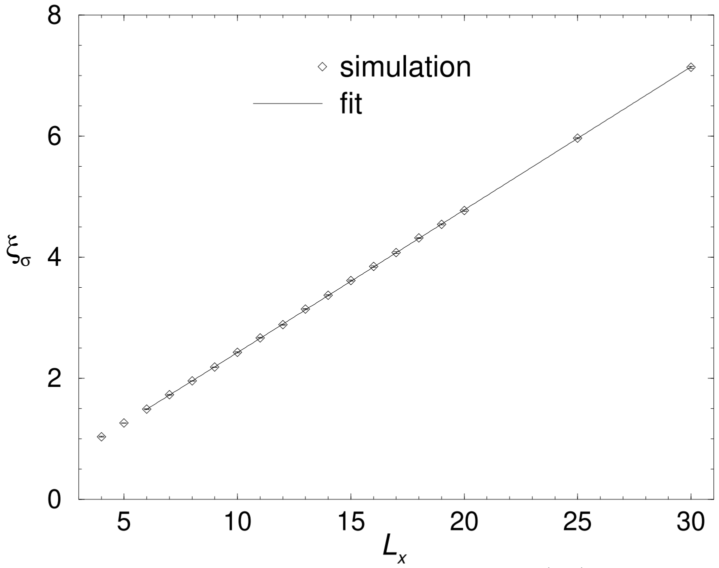

Fig. 1: FSS plot for the spin correlation length $\xi_\sigma(L_x)$ of the 3D Ising model with antiperiodic boundary conditions. The solid line represents a least-square fit according to Eq. (5).

they can be further improved by applying a zero momentum mode projection, i.e., by summing up the values for the densities in the layers $z = \text{const}$ before correlating them [12].

For extracting the correlation lengths from (3) one can cancel out deviations that arise from inaccuracies in the determination of the disconnected parts of the correlation functions and eliminate the need for a correct normalization of the estimates by considering the following set of estimators:

$$\hat{\xi}_i = \Delta \left[\ln \frac{\hat{G}^{c,\|}(i) - \hat{G}^{c,\|}(i-\Delta)}{\hat{G}^{c,\|}(i+\Delta) - \hat{G}^{c,\|}(i)} \right]^{-1}, \tag{4}$$

where $\Delta \geq 1$ should usually be chosen so that a constant drop of $G(i)$ between the pairs of considered points is guaranteed. Variances and cross-correlations of the $\hat{\xi}(i)$ were estimated using a combined binning [13] and jackknifing [14] technique. In a process of statistical optimization, resulting in the leaving out of the corrupt estimates $\hat{\xi}(i)$ for distances in the regions $i < \Delta$ and $i > L_z/2$, one ends up with a final value for the correlation lengths ξ_σ and ξ_ϵ of the considered system.

All simulations were done at inverse temperatures, which were either highly precise single estimates of the inverse critical temperature of the bulk model or weighted means of several such estimates [15, 16], the influence of uncertainties in these values being checked via a temperature reweighting technique.

4 Results

The cumulated estimates for the correlation lengths $\hat{\xi}(L_x)$ for the different system sizes exhibit an almost perfect linear scaling behavior as shown in Fig. 1 for the Ising

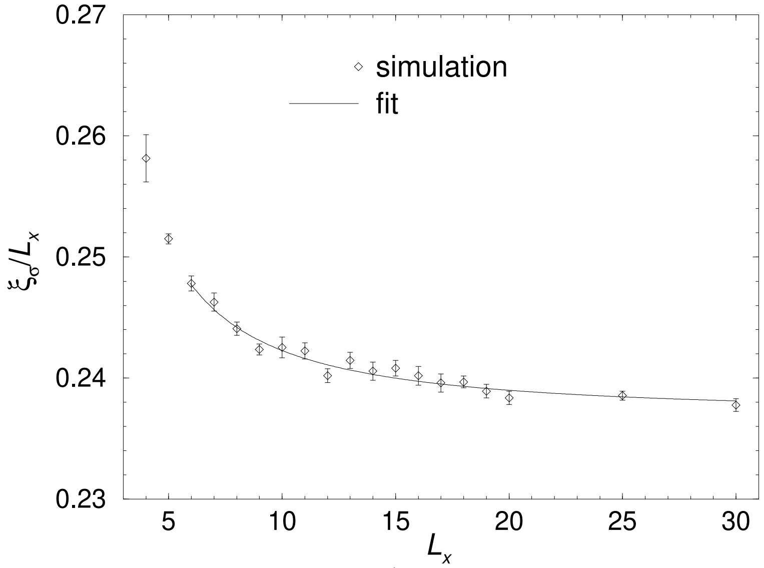

Fig. 2: Scaling of the amplitudes ξ_σ/L_x of the 3D Ising model with antiperiodic boundary conditions.

model and antiperiodic bc. For all models we analyzed system sizes between $L_x = 4$ and 30 and volumes up to about $3 \cdot 10^5$ spins. The plot of the amplitudes $\hat{\xi}/L_x$ in Fig. 2, however, reveals a clear resolution of corrections to scaling, however. Therefore fits to a law including corrections of the form

$$\xi(L_x) = AL_x + BL_x^\alpha \tag{5}$$

were done to arrive at estimates for the leading order scaling amplitudes A_σ and A_ϵ. The final results for these leading amplitudes are summarized in Table 1. The values for the scaling dimensions shown for comparison are once again weighted literature means [7].

5 Conclusions

The clear conclusion of these results for all three models under consideration is that, while for the generic case of periodic bc the ratios of the amplitudes and the scaling dimensions differ by at least about thirty sigma, in the case of *antiperiodic* bc both ratios agree to a very high level of precision, thus giving the conjecture of a law equivalent to (1) for 3D models enough backing to think seriously about a theoretical justification. So, for the $n = 1, 2, 3$ representatives of the class of O(n) spin models one can state that the finite-size scaling amplitude ratios of the the correlation lengths of the magnetization and energy densities is determined by the corresponding scaling dimensions and thus universal; in connection with additional results for the case $n = 10$ [16] and an analytical results for the spherical model [17], it seems reasonable to assume that such a relation holds for the whole class of O(n) spin models. Note, however, that the amplitude A in Eq. (1), which was $1/2\pi = \text{const}$ in the 2D case, does now depend on the model under consideration, i.e., the dimension n of the order parameter [15].

Table 1: Finite-size scaling amplitudes of the correlation lengths of the Ising, XY, and Heisenberg models on the $T^2 \times \mathrm{I\!R}$ geometry.

model		pbc	apbc
Ising	A_σ	0.8183(32)	0.23694(80)
	A_ϵ	0.2232(16)	0.08661(31)
	A_σ/A_ϵ	3.666(30)	2.736(13)
	x_ϵ/x_σ	2.7326(16)	
XY	A_σ	0.75409(59)	0.24113(57)
	A_ϵ	0.1899(15)	0.0823(13)
	A_σ/A_ϵ	3.971(32)	2.930(47)
	x_ϵ/x_σ	2.923(7)	
Heisenberg	A_σ	0.72068(34)	0.24462(51)
	A_ϵ	0.16966(36)	0.0793(20)
	A_σ/A_ϵ	4.2478(92)	3.085(78)
	x_ϵ/x_σ	3.091(8)	

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