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Numerical extension of CFT amplitude universality to three-dimensional systems

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Abstract

Conformal field theory (CFT) predicts universal relations between scaling amplitudes and scaling dimensions for two-dimensional systems on infinite length cylinders, which hold true even independent of the model under consideration. We discuss different possible generalizations of such laws to three-dimensional geometries. Using a cluster update Monte Carlo algorithm we investigate the finite-size scaling (FSS) of the correlation lengths of several representatives of the class of three-dimensional classical O(n) spin models. We find that, choosing appropriate boundary conditions, the two-dimensional situation can be restored. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Augmenting the scale invariance of a system of statistical mechanics at a critical point, which leads to the theory of the renormalization group (RG), by the additional symmetries of rotational, translational and inversion invariance is a powerful tool for the understanding of critical systems, especially in two dimensions (2D), where the group of those *conformal* symmetry transformations becomes infinite dimensional [1,2]. As a consequence, conformal field theory (CFT) provides a complete (continuum) solution of critical systems in 2D, in particular comprising finite-size scaling (FSS) laws *including the amplitudes*. As an example of the latter, consider the logarithmic map

$$w = \frac{L}{2\pi} \ln z, \quad z \in \mathbb{C} \tag{1}$$

in the complex plane $z = (z, \bar{z})$, which wraps the plane around a cylinder of infinite length and circumference L, i.e. the geometry $S^1 \times \mathbb{R}$. Since this map is conformal,

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it gives the transformation of the critical two-point correlation function of a primary operator ϕ [3,4]. In the limit of large distances in the infinite direction this implies a longitudinal correlation length of

$$\xi_{||} = \frac{L}{2\pi x}, \tag{2}$$

with x being the scaling dimension of ϕ. Note the triple universality in this relation: (i) within a certain conventional universality class and for a fixed operator the scaling amplitude of the corresponding correlation length should be the same for all models; (ii) moreover, for a certain model all operator-dependent information should be condensed in the corresponding scaling dimension with an overall fixed amplitude of $1/2\pi$; (iii) finally, relation (2) is meant to hold for models of an arbitrary universality class, as long as they exhibit critical behavior (and have short-ranged interactions). In the case of the lattice Ising model Eq. (2) has been numerically checked [5] and, moreover, coincides with the leading term of the Onsager solution for $\xi_\sigma(L)$ [6]. Specializing on the local densities of magnetization and energy, which are the only primary operators in the 2D Ising universality class, their correlation length ratio becomes $\xi_\sigma/\xi_\varepsilon = x_\varepsilon/x_\sigma$. Changing the periodic boundary conditions (*pbc*) along the strip to an *antiperiodic* boundary (*apbc*) destroys most of this "hyper" universality: for the case of a nearest-neighbor Ising model one ends up with $\xi_\sigma = 4\pi L/3$, $\xi_\varepsilon = \pi L/4$ [1,2]. Thus, the universality aspects (ii) and (iii) above get lost and (i) gets restricted.

A direct generalization of these results to physically more appealing higher-dimensional systems is hindered by the fact that the conformal group becomes finite dimensional for spacial dimensions $d \geqslant 3$; however, since the logarithmic map (1) does not make use of the full CFT theory, some generalization to higher dimensions is possible. In polar coordinates it only affects the radial part, but leaves the angular part of the coordinates invariant. Thus, mapping $\mathbb{R}^d$ to the space $S^{d-1} \times \mathbb{R}$, Cardy [2] arrived at the relation

$$\xi = \frac{R}{x}, \tag{3}$$

where R is the radius of S^{d-1}. This generalized mapping is still conformal; it has to be noted, however, that it connects *different* geometries for $d \geqslant 3$ instead of being a meromorphism acting on the Riemann sphere. Thus, for dimensions greater than two the meaning of a *primary* operator in this context is not clear, so that this result should be considered a conjecture. Numerical studies of this problem are hampered by the difficulty to regularly discretize the curved spaces S^{d-1}. A first attempt to establish this result numerically for $d = 3$ and the Ising model in the Hamiltonian limit used Platonic solids as approximation of S^2 and was inconclusive due to the very limited size of these polyhedra [7]. Another possible generalization leads to the geometry $S^1 \times \cdots \times S^1 \times \mathbb{R}$, which is more easily accessible for numerical studies, but is not related to a flat space via a conformal transformation. In a transfer matrix study of the Ising model in the Hamiltonian limit on the three-dimensional (3D) manifold $S^1 \times S^1 \times \mathbb{R} \equiv T^2 \times \mathbb{R}$, Henkel [8,9] found for the correlation length ratio of spin and energy densities the values $\xi_\sigma/\xi_\varepsilon = 3.62(7)$ for *pbc* and $\xi_\sigma/\xi_\varepsilon = 2.76(4)$ for *apbc*, which compared to the ratio of scaling dimensions of $x_\varepsilon/x_\sigma = 2.7326(16)$ seemed to indicate that changing the boundary conditions along the torus directions from *pbc* to *apbc* could restore the 2D result, in qualitative agreement with a Metropolis Monte Carlo (MC) study [10]. These 3D observations form a possible starting point for a generalization of CFT methods to higher-dimensional systems. Here, we discuss numerical analyses focusing on the influence of boundary conditions on the validity of scaling laws of the form (2) and the question, which degree of universality according to the above described classification scheme can be retained for 3D systems.

2. Systems with spherical cross section

2.1. Model and lattice

We consider an O(n) symmetric classical spin model with nearest-neighbor, ferromagnetic interactions in zero field with Hamiltonian

$$\mathscr{H} = -J \sum_{\langle ij \rangle} \sigma_i \, \sigma_j, \quad \sigma_i \in S^{n-1}, \tag{4}$$

specializing on the Ising case $n = 1$ on the 3D geometry $S^2 \times \mathbb{R}$. Because the Platonic solids as triangulations of the sphere contain only up to 20 points, one has to switch to slightly irregular discretizations of the sphere. The model lattice that suggests itself in the first place is a square mesh on a cube [11], which we call lattice (C). Its main anomaly consists in the defective coordination numbers of the corner points and the concentration of the curvature of the lattice around the cube edges. The former could be amended by the insertion of triangles in place of the cube corners, while a smearing out of the spherical curvature can be accomplished by projecting the cube on the sphere, resulting in geometry (S). As found in Ref. [11] for bulk quantities, however, differences in the scaling behavior between lattices (C) and (S) are quite small. Furthermore, there is evidence to believe that *ratios* of correlation lengths of primary operators are universal [8,9,12–14], so that we can expect good agreement regardless of the lattice used if Cardy's conjecture, Eq. (3), holds. Finally, choosing lattices with differing sorts and degrees of defects might function as an explicit test of universality. Here we concentrate on the cube discretization (C) of the sphere, which consists of six $L_x \times L_x$ square lattices. Discretization (S) will be considered elsewhere [15]. For the approximate sphere discretizations there is some ambiguity in the definition of the radius R of the sphere a given cube lattice with edge lengths L_x should correspond to. Defining the sphere radius through $R = \sqrt{S/4\pi}$, the lattice surface S could be defined by counting the number of sites, bond pairs or elementary squares, respectively, leading to areas

$$S = \begin{cases} 6L_x(L_x - 2) + 8 \text{ “sites”}, \\ 6L_x(L_x - 2) + 6 \text{ “bonds”, “squares”} \end{cases} \tag{5}$$

and thus generating two different sorts of pseudo radii, which only differ by the constant shift in Eq. (5), thus leading to slightly different FSS approaches.

2.2. Simulation and results

We used a single cluster update MC algorithm for all of the simulations reported. Motivated by the fact that the densities of magnetization and energy are primary in the case of the 2D Ising model we concentrated on those two observables for the 3D systems also. Thus, candidates for measurements are their connected correlation functions $G_\sigma^c(\mathbf{x}_1,\mathbf{x}_2)$ and $G_\varepsilon^c(\mathbf{x}_1,\mathbf{x}_2)$. Since we are interested in the correlations along the infinite $\mathbb{R}$-direction (the z-direction in the discrete case) only, the variance of these estimators can be reduced by averaging over estimates $\hat{G}^c(\mathbf{x}_1,\mathbf{x}_2)$ such that $(\mathbf{x}_1-\mathbf{x}_2)\,||\,\hat{e}_z$ and $i\equiv|\mathbf{x}_1-\mathbf{x}_2|=\text{const}$, resulting in estimates $\hat{G}^{c,||}(i)$. A further improvement can be achieved by considering a zero-momentum projection, i.e., using averages over layers $z=\text{const}$ and evaluating correlation functions of these layer variables [5]. Due to the statistical character of a MC simulation, one has to assume a long-distance behavior of the correlation functions of the form $\hat{G}^{c,||}(i)=a\exp(-i/\xi)+b$, including a residual term b. Since extracting the correlation length from this relation involves an intrinsically unstable non-linear three-parameter fit, we decided instead to use an estimator for the correlation length that systematically eliminates the multiplicative and additive constants a and b:

$$\hat{\xi}_i=\Delta\left[\ln\frac{\hat{G}^{c,||}(i)-\hat{G}^{c,||}(i-\Delta)}{\hat{G}^{c,||}(i+\Delta)-\hat{G}^{c,||}(i)}\right]^{-1}, \tag{6}$$

the distance $\Delta\geqslant 1$ forming an additional free parameter of the estimation. Given Eq. (6), final estimates for the correlation lengths are formed by averaging over the estimates $\hat{\xi}_i$ within a regime of distances i that is confined by short-distance lattice artifacts and the effect of the finite length L_z. Final error estimates are evaluated using the jackknife resampling technique [16], which was also used to check for and reduce the statistical bias of estimators (6) [5]. Traversing the above described steps in the determination of correlation lengths one arrives at a FSS sequence of estimates $\xi_{\sigma/\varepsilon}$ for the Ising model as depicted in Fig. 1(a). Since Fig. 1(b) reveals that corrections to scaling are resolvable one has to use non-linear fits of the form

$$\xi(R)=AR+BR^\alpha\,, \tag{7}$$

including the effective correction exponent α as a free parameter. We thus arrive at final estimates for the leading FSS amplitudes of $A_\sigma=1.996(20)$ and $A_\varepsilon=0.710(38)$, which agree quite well with the conjectured amplitudes of $A_\sigma^{\text{conj}}=1/x_\sigma=1.9324(19)$ and $A_\varepsilon^{\text{conj}}=1/x_\varepsilon=0.70711(35)$. Finally, comparing the measured amplitude *ratio* of $A_\sigma/A_\varepsilon=2.81(15)$ with the conjectured one of $x_\varepsilon/x_\sigma=2.7326(16)$ we find nice agreement as well. So, our results imply that for the $S^2\times\mathbb{R}$-geometry the same degree of universality as in 2D is obeyed. The fact that the quite crude approximation (C) to the sphere gives correct results even for the amplitudes, is quite strong evidence for their universality. It would

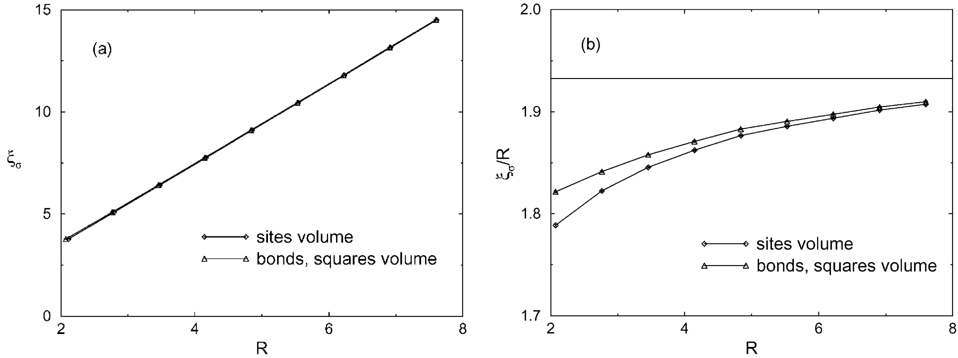

Fig. 1. (a) FSS plot for the spin correlation length $\xi_\sigma(R)$. (b) Scaling of the amplitudes ξ_σ/R. The horizontal line indicates the conjectured amplitude.

Table 1
Correlation length amplitudes of the Ising, XY, and Heisenberg models on $T^2 \times \mathbb{R}$

n		A_σ	A_ε	A_σ/A_ε	x_ε/x_σ	A
	pbc	0.8183(32)	0.2232(16)	3.666(30)		
1					2.7326(16)	
	apbc	0.23694(80)	0.08661(31)	2.736(13)		0.12262(43)
	pbc	0.75409(59)	0.1899(15)	3.971(32)		
2					2.923(7)	
	apbc	0.24113(57)	0.0823(13)	2.930(47)		0.12486(47)
	pbc	0.72068(34)	0.16966(36)	4.2478(92)		
3					3.091(8)	
	apbc	0.24462(51)	0.0793(20)	3.085(78)		0.12625(49)

be interesting to test this universality with even more distorted discretizations like the "pillow"-geometry of Ref. [11] and to check if it also holds for other universality classes.

3. Systems with toroidal cross section

The effect of boundary conditions on the behavior of the scaling law was studied in the geometry $T^2 \times \mathbb{R}$, which in contrast to $S^2 \times \mathbb{R}$ is not conformally flat. Simulations were done on $L_x \times L_y \times L_z$ lattices with $L_x = L_y$ and *pbc* or *apbc* in the x and y directions applied. To be able to check for the most general universality (iii) above we choose different dimensions of the order parameter in Eq. (4), thus analyzing the Ising ($n=1$) model as well as the XY ($n=2$) and Heisenberg ($n=3$) models [13,14]. Fitting the estimates for the correlation lengths with ansatz (7), we arrive at the scaling amplitudes listed in Table 1. In all three cases we obtain excellent agreement between A_σ/A_ε and x_ε/x_σ in the case of the *apbc* systems and a clear divergence when choosing

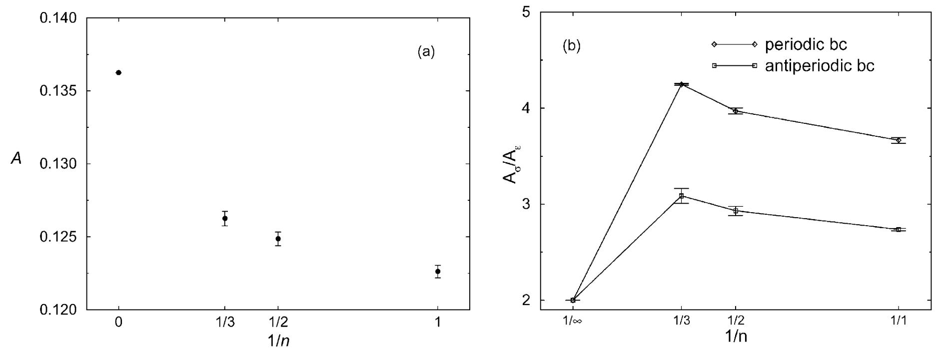

Fig. 2. (a) Amplitudes A of the relation $\xi = Ax^{-1}L$ versus the inverse dimension of the order parameter $1/n$. (b) Ratio of the scaling amplitudes A_σ and A_ε.

pbc. This underscores type (iii) universality for this relation. Furthermore, an analytical study for the case of the spherical model, whose partition function coincides with the $n \to \infty$ limit, also obeys Eq. (2) in the case of *apbc* [13]. Since the systems with *apbc* obey a scaling law of the form $\xi(L_x) = A/x \cdot L_x$, it is of further interest to study the behavior of the operator independent "meta"-amplitude A, which is $1/2\pi$ in the case of the systems with spherical cross section in 2D and 3D (with $L_x = 2\pi R$). This amplitude is inaccessible for the transfer matrix approach since the corresponding quantum Hamiltonian is only defined up to an overall normalization. Using the amplitudes $A_\sigma = A/x_\sigma$ to determine A and $x_\sigma = 0.5175(5)$, $0.5178(15)$ and $0.5161(17)$ for the Ising, the XY and the Heisenberg model, respectively, we arrive at the values listed in Table 1. Plotting these amplitudes as a function of the order-parameter dimension n reveals that they, in contrast to the 2D case, in fact vary with n and thus universality of type (iii) is lost for the $T^2 \times \mathbb{R}$ systems, cf. Fig. 2(a). Notice that the amplitude $A \approx 0.13624$ [17–19] for the spherical model fits well into the variation encountered for finite n. Plotting the amplitude ratios A_σ/A_ε, on the other hand, shows the expected behavior for finite n, but an astonishing jump between the eye-ball extrapolation for $n \to \infty$ and the spherical model result, cf. Fig. 2(b). Since we know from the $1/n$ expansion that critical exponents vary smoothly and monotonically with n, for the $n \to \infty$ limit it is neither plausible that the amplitude ratios of the systems with *pbc* and *apbc* should coincide, nor that one of the two ratios should approach the value 2 of the spherical model. Instead one would expect the ratios to converge to a value around 4 in the case of the *apbc* and about 6 for *pbc*. This view is supported by further results for the $n = 10$ case [15], which match the eye-ball extrapolation. Comparing Fig. 2(a) with (b) it becomes clear that this discontinuous behavior must be entirely due to the variation of the energy amplitude A_ε. And indeed, directly evaluating the scaling dimension of the energy density in the spherical model results in $x_\varepsilon = 1$ [17–19], which together with $x_\sigma = \frac{1}{2}$ makes up a ratio of 2; using the scaling relation $x_\varepsilon = (1 - \alpha)/\nu$, on the other hand, with $\nu = 1$ and $\alpha = -1$ suggests $x_\varepsilon/x_\sigma = 4$, coinciding with the expectation for the $n \to \infty$ limit. This behavior might be connected to the asymmetry of the specific heat around the critical point in the spherical model [20]: below T_c a constant C_v $(\alpha = 0)$ suggests $x_\varepsilon = 1$, while above T_c a cusp singularity with $\alpha = -1$ would result in $x_\varepsilon = 2$. Thus, the discontinuity could be explained with a vanishing amplitude of the specific-heat singularity below T_c that could be interpreted as effectively resulting in a vanishing exponent $\alpha = 0$. More analytical work is necessary to fully understand this subtle point.

4. Conclusions

Using a high-precision single-cluster MC method, we examined possible extensions to 3D geometries of a prominent scaling law involving the amplitudes that can be proven analytically in 2D. For the 3D geometry $S^2 \times \mathbb{R}$ we find Cardy's conjecture (3) to hold for the Ising model, specializing on the operators primary in 2D. There is no reason to believe for this 3D case in a deviation from the full degree of "hyper"-universality found in 2D. Dropping the condition of conformal flatness and thus loosing any direct connection to CFT methods, scaling law (2), nevertheless, can be retained on the geometry $T^2 \times \mathbb{R}$ when changing the boundary conditions from the usual *pbc* case to *apbc*, as explicitly checked for the Ising, XY and Heisenberg models. The degree of universality in this case, however, is restricted to the aspects (i) and (ii) above (aspect (i) is discussed in Refs. [8,9,12]). The overall "meta"-amplitude A gets, in contrast to the 2D case, model dependent as shown for the class of $O(n)$ spin models. Comparing this variation with an analytical result for the spherical model we encounter a discrepancy that makes it unplausible that the $n \to \infty$ limit of the $O(n)$ model coincides with the spherical model in this respect. Thus, the widely used notion of "equivalence" between those two models is reduced to the identity of partition functions as originally stated by Stanley [21,22], while observables that cannot be written as derivatives of the partition function do not coincide in all cases. We want to emphasize that there is up to now no theoretical explanation for why changing the boundary conditions from *pbc* to *apbc* should be essential, but in view of the lack of exact results for 3D systems we consider it a rewarding task to explain these observations.

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