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Numerical tests of CFT conjectures for 3D spin systems

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Abstract

One kind of predictions of conformal field theory for two-dimensional systems are universal relations between scaling amplitudes and scaling dimensions on infinite length cylinders. We discuss different possible generalizations of such laws to three-dimensional geometries. Using cluster update Monte Carlo simulations we investigate the finite-size scaling of the correlation lengths of several three-dimensional classical O(n) spin models. We find that, choosing appropriate geometries or boundary conditions, the two-dimensional situation can be restored. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Augmenting the scale invariance of a physical system at a critical point, being the basis of the renormalization group (RG) theory, by the additional symmetries of rotational, translational and inversion invariance has led to a quite complete understanding of two-dimensional (2D) critical phenomena. This comprises in particular finite-size scaling (FSS) laws *including the amplitudes*. Mathematically, the reason for the exceptional predictive power of such symmetry considerations can be traced back to the fact that this group of *conformal* symmetry transformations is infinite-dimensional in 2D [1]. As an example of the FSS predictions of conformal field theory (CFT), consider the logarithmic map $w = (L/2\pi)\ln z$, $z \in \mathbb{C}$, which wraps the complex plane around a cylinder of infinite length and circumference L, i.e. the geometry $S^1 \times \mathbb{R}$. Being conformal, this map gives the full expression of the critical two-point correlation function of a primary operator ϕ on $S^1 \times \mathbb{R}$ [2], implying in the limit of large distances in the infinite direction a longitudinal correlation length of

$$\xi_{\parallel} = \frac{L}{2\pi x}, \tag{1}$$

with x being the scaling dimension of ϕ. This relation exhibits three different aspects of universality:

(i) the scaling amplitude of the correlation length of a given operator should be the same for all models within a universality class;
(ii) all operator-dependent information should be condensed in the associated scaling dimension x with an overall amplitude of $1/2\pi$;
(iii) the relation should hold for models of an arbitrary universality class, as long as they exhibit critical behaviour (and have short-ranged interactions).

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Specializing on the local densities of magnetization and energy, which are the only primary operators in the 2D Ising universality class, their correlation lengths ratio becomes $\xi_\sigma/\xi_\epsilon = x_\epsilon/x_\sigma$. Changing the periodic (p) boundary conditions (bc) along the strip to *antiperiodic* (a) bc destroys most of the "hyper"-universality: for the nearest-neighbor Ising model one ends up with $\xi_\sigma = 4\pi L/3$, $\xi_\epsilon = \pi L/4$ [1]. Thus, the universality aspects (ii) and (iii) above get lost and (i) gets restricted.

A direct generalization of these results for 2D systems to higher dimensions is hindered by the fact that the conformal group becomes finite-dimensional for dimensions $d \geqslant 3$. Observing, however, that the logarithmic map above does not make use of the full CFT, some generalizations to higher dimensions become possible. In polar coordinates the logarithmic map 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] conjectured the relation

$$\xi = \frac{R}{x}, \tag{2}$$

where R is the radius of S^{d-1}. This generalized mapping is still conformal, but for $d \geqslant 3$ it connects *different* geometries instead of being a meromorphism acting on the Riemann sphere. Therefore, for $d \geqslant 3$ the meaning of a *primary* operator in this context is not clear and the relation (2) 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 [3] to establish this result numerically for $d = 3$ and the Ising model in the Hamiltonian limit used Platonic solids as an approximation of S^2, but was inconclusive due to the very limited size of these polyhedra.

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 [4] found for the correlation lengths ratio of spin and energy densities the values $\xi_\sigma/\xi_\epsilon = 3.62(7)$ for p-bc and $\xi_\sigma/\xi_\epsilon = 2.76(4)$ for a-bc, which compared to the ratio of scaling dimensions of $x_\epsilon/x_\sigma = 2.7326(16)$ seemed to indicate that changing the boundary conditions along the torus directions from p-bc to a-bc could restore the 2D result, in qualitative agreement with a Metropolis Monte Carlo (MC) study [5]. 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 and special geometries on the validity of scaling laws of the form (1) and (2), respectively, and the question of what degree of universality according to the above-described classification scheme can be retained for 3D systems.

2. Models and computational tools

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

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\cdot\sigma_j,\quad \sigma_i\in S^{n-1}. \tag{3}$$

The spins σ_i live on the sites of lattices representing the geometries (a) $T^2\times\mathbb{R}$ and (b) $S^2\times\mathbb{R}$ to be described in more detail below. The MC simulations are performed with the Wolff single cluster update algorithm [6]. In the case of a-bc along the torus directions we make use of the equivalence of an antiperiodic boundary to the insertion of a seam of anti-ferromagnetic bonds along the boundary which is straightforward to implement for nearest-neighbor interactions.

The main observables of our simulations are the connected correlation functions of the magnetization and energy densities:

$$\begin{aligned} G_\sigma^c(\mathbf{x}_1,\mathbf{x}_2) &= \big\langle\sigma(\mathbf{x}_1)\cdot\sigma(\mathbf{x}_2)\big\rangle - \langle\sigma\rangle\cdot\langle\sigma\rangle,\\ G_\epsilon^c(\mathbf{x}_1,\mathbf{x}_2) &= \big\langle\epsilon(\mathbf{x}_1),\epsilon(\mathbf{x}_2)\big\rangle - \langle\epsilon\rangle\langle\epsilon\rangle. \end{aligned} \tag{4}$$

Here we defined the local energy density as a sum over the neighborhood of a spin:

$$\epsilon(\mathbf{x}) = -\frac{J}{2}\sum_{\mathbf{x}'\,\mathrm{nn}\,\mathbf{x}}\sigma(\mathbf{x})\cdot\sigma(\mathbf{x}'), \tag{5}$$

the factor $1/2$ ensuring that $E = \sum_\mathbf{x}\epsilon(\mathbf{x})$. It is straightforward to construct a bias-reduced estimator for the case of $(\mathbf{x}_2-\mathbf{x}_1)\parallel\widehat{e}_z$, corresponding to the correlation length $\xi = \xi_\parallel$ in the long direction: first, taking advantage of the translation invariance of the systems along the z-axis (established by periodic boundary conditions along z), one can average over the "layers" $i \equiv |z_2 - z_1| =$ const. To improve on that consider a "zero-mode projection" [7], i.e. define layered variables

$$\overline{\mathcal{O}}_t(z) = \frac{1}{L_x L_y} \sum_{\mathbf{x}', z'=z} \mathcal{O}_t(\mathbf{x}'), \tag{6}$$

where $\mathcal{O}_t = \sigma_t$ or ϵ_t denotes the times series of MC measurements, and consider the estimator

$$\widehat{G}^{c,\parallel}_{\mathcal{O}}(i) = \frac{1}{T}\sum_{t=1}^{T} \frac{1}{L_z} \sum_{|z_2-z_1|=i} \overline{\mathcal{O}}_t(z_1)\overline{\mathcal{O}}_t(z_2) - \left(\frac{1}{TL_z}\sum_{t=1}^{T}\sum_{z} \overline{\mathcal{O}}_t(z)\right)^2, \tag{7}$$

where T denotes the length of the MC time series. This estimator obviously does not directly measure $G^{c,\parallel}$, but inspecting the continuum expression reveals that the deviation stemming from transversal cross-correlations entering the estimator declines exponentially with increasing longitudinal distance i and thus becomes irrelevant in the long-distance limit.

While periodic boundary conditions in the z-direction eliminate surface effects associated with this direction, there are still effects of finite L_z which result in deviations from the $L_z \to \infty$ limit assumed in Eq. (1). In the limit of distances $i \gg \xi_\parallel$ one expects longitudinal correlations according to

$$G^{c,\parallel}(i) \propto \mathrm{e}^{-i/\xi_\parallel} + \mathrm{e}^{-(L_z - i)/\xi_\parallel}. \tag{8}$$

Thus, using too small values of L_z results in an effective underestimation of correlation lengths. In order to keep this effect small enough (assuming $\xi_\parallel \propto L_x$), one has to keep the ratio $L_z/\xi_\parallel \propto L_z/L_x$ fixed, i.e. one has to scale L_z proportionally to L_x. Guided by a comparative study of the 2D Ising model we worked for the 3D systems with $L_z \approx 15\xi_\parallel$, where always the greater correlation length ξ_σ was used in this *a priori* estimate.

In all simulations we controlled the efficiency of the cluster update algorithm by measuring integrated autocorrelation times τ_{int} using a binning technique. Since measurements of $\widehat{G}^{c,\parallel}$ are computationally expensive compared to update steps, measurements were done with frequencies of about $1/\tau_{\mathrm{int}}$.

Having sampled correlation functions according to Eq. (7) and assuming the functional form $G^{c,\parallel}(i) = a\exp(-i/\xi_\parallel) + b$, we refrain from using intrinsically unstable non-linear three-parameter fits and resort to the following estimator instead,

$$\widehat{\xi}_{\mathcal{O}}(i) = \Delta\left[\ln\frac{\widehat{G}^{c,\parallel}_{\mathcal{O}}(i) - \widehat{G}^{c,\parallel}_{\mathcal{O}}(i-\Delta)}{\widehat{G}^{c,\parallel}_{\mathcal{O}}(i+\Delta) - \widehat{G}^{c,\parallel}_{\mathcal{O}}(i)}\right]^{-1}, \tag{9}$$

which eliminates both the additive and multiplicative constants a and b above. Apart from stability considerations this approach simplifies the distinction of the short- and long-distance regimes. The parameter Δ in Eq. (9) can be used to optimize the signal-noise ratio for the correlation length estimate. Here, we used $\Delta \approx 2\xi_\epsilon$ for both estimators $\widehat{\xi}_\sigma(i)$ and $\widehat{\xi}_\epsilon(i)$.

The estimation of statistical errors (variances) of complex, non-linear combinations of observable measurements like in Eq. (9) requires some care. Temporal correlations can be eliminated by forming subaverages of length μ ("binning"), i.e. by using reduced time series of length $T' = T/\mu$. In our runs the bin size was always several thousand measurements. To cope with the non-linearities in Eq. (9) we use resampling techniques such as the "jackknife" [8] which mimic the brute force error estimation method of comparing k completely independent MC time series of lengths T' and applying the naive estimates: removing single elements (i.e. bins) of a single time series of length T' one by one results in T' time series of length $T' - 1$, e.g., for the correlation function estimates:

$$\widehat{G}_{(s)}(i) = \frac{1}{T'-1}\sum_{t\neq s} \widehat{G}_t(i), \tag{10}$$

resulting in jackknife-block estimates for the correlation length of:

$$\begin{aligned} \widehat{\xi}_{(s)}(i) &= \Delta\left[\ln\frac{\widehat{G}_{(s)}(i) - \widehat{G}_{(s)}(i-\Delta)}{\widehat{G}_{(s)}(i+\Delta) - \widehat{G}_{s}(i)}\right]^{-1}, \\ \widehat{\xi}_{(\cdot)}(i) &= \frac{1}{T'}\sum_{s} \widehat{\xi}_{(s)}(i). \end{aligned} \tag{11}$$

Then the jackknife estimate of variance is given by:

$$\widehat{\mathrm{VAR}}\big(\widehat{\xi}(i)\big) = \frac{T'-1}{T'}\sum_{s=1}^{T'}\big(\widehat{\xi}_{(s)}(i) - \widehat{\xi}_{(\cdot)}(i)\big)^2. \tag{12}$$

Note the missing factor of $1/(T'-1)^2$ as compared to the usual variance estimate which accounts for the trivial correlation between the T' jackknife-block estimates.

An improved final estimate can be achieved by an average over the $\widehat{\xi}(i)$, $i = i_{\min}, \ldots, i_{\max}$. When correlations between the individual estimates are negligible, the usual recipe is averaging over the estimates $\widehat{\xi}(i)$ with weights $\alpha_i \propto 1/\sigma^2(\widehat{\xi}(i))$ that minimize the theoretical variance of the average. Here, however, cross-correlations between adjacent estimates $\widehat{\xi}(i)$ cannot be neglected (they increase with increasing Δ) and one has to choose the weights according to

$$\alpha_k = \frac{\sum_i (\Gamma^{-1})_{ik}}{\sum_{i,j} (\Gamma^{-1})_{ij}}, \tag{13}$$

in order to minimize the variance of the average, as can be proven by a simple variational calculation. Here, Γ denotes the covariance matrix of the $\widehat{\xi}(i)$ which can be estimated within the jackknife resampling scheme as:

$$\begin{aligned} \widehat{\mathrm{CORR}}_{ij} &\equiv \widehat{\mathrm{CORR}}\big(\widehat{\xi}(i), \widehat{\xi}(j)\big) \\ &= \frac{T'-1}{T'} \sum_{s=1}^{T'} \big(\widehat{\xi}_{(s)}(i) - \widehat{\xi}_{(\cdot)}(i)\big) \\ &\quad \times \big(\widehat{\xi}_{(s)}(j) - \widehat{\xi}_{(\cdot)}(j)\big). \end{aligned} \tag{14}$$

The fact that, considering Eq. (13), variance and covariance estimates directly influence the final results for the correlation lengths, gave the motivation for the quite careful statistical treatment presented above.

3. Systems with toroidal cross section

Let us first consider the toroidal 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 p-bc or a-bc in the x- and y-directions. To be able to check for the most general universality (iii) above we chose different parameters n of the O(n) symmetry group of the Hamiltonian (3), thus analyzing the Ising ($n = 1$), XY ($n = 2$), Heisenberg ($n = 3$), and $n = 10$ models [9,10]. When fitting the scaling behaviour (1) to the measured correlation lengths we accounted for corrections to scaling by using the ansatz

$$\xi_{\sigma/\epsilon}(L_x) = A_{\sigma/\epsilon} L_x + B_{\sigma/\epsilon} L_x^{\kappa}, \tag{15}$$

where $\kappa < 1$ is an effective correction exponent. This yields the scaling amplitudes listed in Table 1. In all cases we obtain excellent agreement of A_σ/A_ϵ with x_ϵ/x_σ in the case of a-bc systems and a clear overshooting for p-bc which, however, is remarkably well described by an empirical factor of 4/3 [10]. For the a-bc systems this underscores type (ii) universality of the scaling relation.

Table 1
Correlation length amplitudes of the Ising, XY, Heisenberg, and $n = 10$ models on $T^2 \times \mathbb{R}$

n		A_σ	A_ϵ	A_σ/A_ϵ	x_ϵ/x_σ
1	p	0.8183(32)	0.2232(16)	3.666(30)	2.7264(13)
	a	0.23694(80)	0.08661(31)	2.736(13)	
2	p	0.75409(59)	0.1899(15)	3.971(32)	2.9136(38)
	a	0.24113(57)	0.0823(13)	2.930(47)	
3	p	0.72068(34)	0.16966(36)	4.2478(92)	3.0891(79)
	a	0.24462(51)	0.0793(20)	3.085(78)	
10	p	0.671107(59)	0.1350(23)	4.971(83)	3.615(70)
	a	0.25865(46)	0.0710(11)	3.645(55)	

It is of further interest to study the behaviour of the operator-independent "meta"-amplitude $A = x_\sigma A_\sigma = x_\epsilon A_\epsilon$, which is inaccessible for the transfer matrix approach since the corresponding quantum Hamiltonian is only defined up to an overall normalization. Using our estimates for A_σ and $x_\sigma = 0.5182(4)$, 0.5188(9), 0.5160(17), and 0.512(12) for the Ising, XY, Heisenberg, and $n = 10$ model, respectively, we arrive at the data plotted in Fig. 1(a). We see that the universality of the type (iii) is clearly lost for the $T^2 \times \mathbb{R}$ systems. Notice that the amplitude $A \approx 0.13624$ [11] 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 behaviour for finite n, but a jump between the eye-ball extrapolation for $n \to \infty$ and the spherical model result $A_\sigma/A_\epsilon = 2$, cf. Fig. 1(b). In view of Fig. 1(a) the jump must be entirely due to the variation of the energy amplitude A_ϵ. In fact, while a direct calculation within the spherical model gives $x_\epsilon = 1$ and hence a ratio of $x_\epsilon/x_\sigma = 2$ (using $x_\sigma = 1/2$) [11], the scaling relation $x_\epsilon = (1-\alpha)/\nu$ with $\nu = 1$ and $\alpha = -1$ suggests $x_\epsilon/x_\sigma = 4$ [10,12], coinciding with the $n \to \infty$ extrapolation.

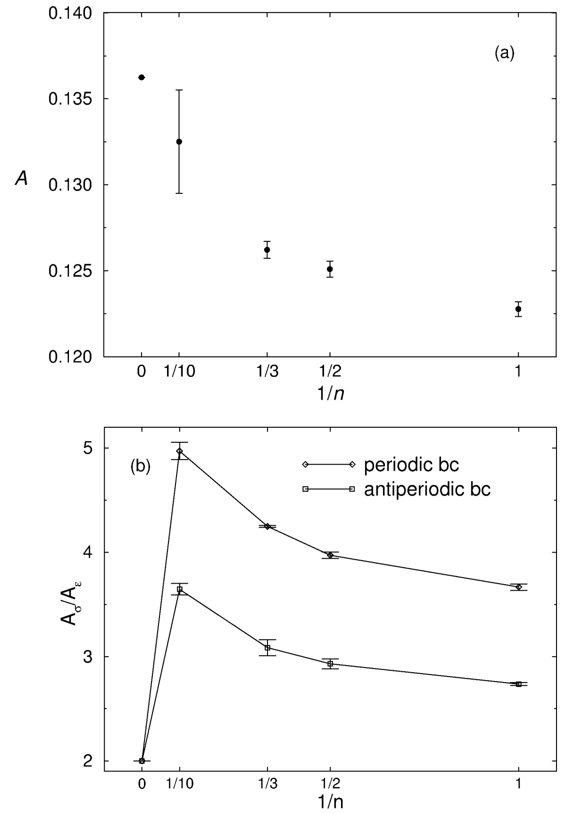

Fig. 1. (a) Amplitudes A of the relation $\xi = Ax^{-1}L$ versus the inverse dimension of the order parameter $1/n$. (b) Ratio of the scaling amplitudes A_σ and A_ϵ.

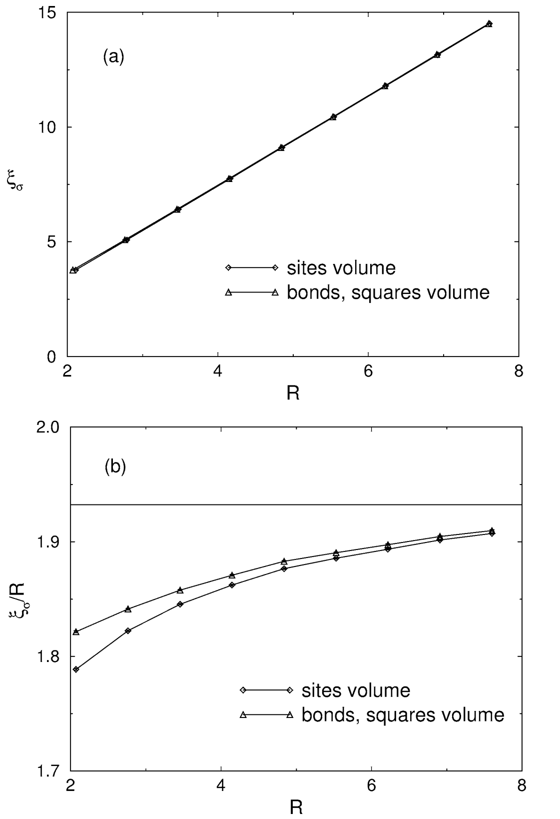

Fig. 2. (a) FSS plot for the spin correlation length $\xi_\sigma(R)$. (b) Scaling of the amplitudes ξ_σ/R. The horizontal line indicates the conjectured amplitude.

4. Systems with spherical cross section

Let us now turn to 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 [13], 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 [13] for bulk quantities, however, differences in the scaling behaviour between lattices (C) and (S) are quite small. Furthermore, there is evidence to believe that *ratios* of correlation lengths of primary operators are universal [4,10,14], so that we can expect good agreement regardless of the specific lattice used if Cardy's conjecture Eq. (2) holds. Here we concentrate on the cube discretization (C) of the sphere, which consists of six $L_x \times L_x$ square lattices [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, leading to areas

$$S = \begin{cases} 6L_x(L_x-2)+8 & \text{“sites”}, \\ 6L_x(L_x-2)+6 & \text{“bonds”, “squares”}, \end{cases} \qquad (16)$$

and thus generating two different sorts of pseudo-radii, which only differ by the constant shift in Eq. (16), thus leading to slightly different FSS approaches.

Traversing the above-described steps in the determination of correlation lengths one arrives at a FSS sequence of estimates $\xi_{\sigma/\epsilon}$ for the Ising model as depicted in Fig. 2(a). Since Fig. 2(b) reveals that corrections to scaling are resolvable, one again has to use non-linear fits of the form (15) (with L_x replaced by R). We thus arrive at final estimates for the leading FSS amplitudes of $A_\sigma = 1.996(20)$ and $A_\epsilon = 0.710(38)$, which agree quite well with the conjectured amplitudes of $A_\sigma^{\text{conj}} = 1/x_\sigma = 1.9301(19)$ and $A_\epsilon^{\text{conj}} = 1/x_\epsilon = 0.70776(25)$. Consequently, comparing the measured amplitude *ratio* of $A_\sigma/A_\epsilon = 2.81(15)$ with the conjectured one of $x_\epsilon/x_\sigma = 2.7269(16)$ 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 be interesting to test this universality with even more distorted discretizations like the "pillow" geometry of Ref. [13] and to check whether it also holds for other universality classes.

5. Conclusions

Using large-scale cluster MC simulations combined with high-precision analyses tools, we examined two 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 (2) 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 losing any direct connection to CFT methods, the scaling law (1) nevertheless can be retained on the geometry $T^2 \times \mathbb{R}$ when changing the boundary conditions from the usual p-bc case to a-bc, as explicitly checked for the Ising, XY, Heisenberg, and $n = 10$ models. In contrast to the 2D case, however, the overall "meta"-amplitude A is model-dependent.

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