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Author post-print (accepted) deposited in CURVE April 2016

Original citation & hyperlink:

Weigel, M. and Janke, W. (2000) Universal amplitude-exponent relation for the Ising model on sphere-like lattices. EPL, volume 51 (5): 578

<http://dx.doi.org/10.1209/epl/i2000-00377-0>

DOI 10.1209/epl/i2000-00377-0

ISSN 0295-5075

ESSN 1286-4854

Publisher: IOP Publishing Ltd

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EUROPHYSICS LETTERS

Europhys. Lett., (), pp. ()

Universal amplitude-exponent relation for the Ising model on sphere-like lattices

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(received ; accepted)

PACS. 75.10Hk – Classical spin models.

PACS. 75.40Mg – Numerical simulation studies.

PACS. 11.25Hf – Conformal field theory, algebraic structures.

Abstract. – Conformal field theory predicts finite-size scaling amplitudes of correlation lengths universally related to critical exponents on sphere-like, semi-finite systems $S^{d-1} \times \mathbb{R}$ of arbitrary dimensionality d . Numerical studies have up to now been unable to validate this result due to the intricacies of lattice discretisation of such curved spaces. We present a cluster-update Monte Carlo study of the Ising model on a three-dimensional geometry using slightly irregular lattices that confirms the validity of a linear amplitude-exponent relation to high precision.

Introduction. – The observation that the symmetry of systems at a critical point goes beyond scale invariance emerging from the divergence of correlation lengths, and additionally comprises rotational and translational as well as inversional invariance has greatly enlarged the scope of exact results that can be derived for such systems on field-theory grounds. While customary scaling theory and the real-space renormalisation ansatz [1, 2] give rise to general relations between the scaling exponents and the concept of universality [3] of exponents and certain amplitude ratios, conformal field theory (CFT) [4, 5] allows for a classification of models according to their operator contents, thus providing the *values* of exponents and amplitude ratios, and, in special cases, even the amplitudes themselves. By interpreting the finite size of a system as an additional field in the scaling ansatz, these considerations apply not only to thermal scaling but as well to the scaling of observables of finite systems at a critical point in the limit of diverging system sizes, *i.e.* to finite-size scaling (FSS) [6]. Concerning universality in FSS, based on renormalisation-group considerations it has been argued that for semi-finite systems below their upper critical dimension the correlation lengths (measured in units of the lattice spacing) themselves are universal quantities [7]. Exploiting conformal invariance this statement can be strengthened and the amplitude of this universal correlation-length scaling

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can be calculated at least for a special geometry. To see this, consider the logarithmic map

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

in two dimensions, which wraps the complex plane \mathbb{C} around an infinite-length cylinder of circumference L . Exploiting the facts that the critical, connected two-point correlation function in the plane is fixed by the postulate of conformal invariance and that the given map is conformal, the critical two-point function of any conformally transforming (primary) operator on the cylinder $S^1 \times \mathbb{R}$ follows immediately. In particular, correlations of the considered operator along the \mathbb{R} -axis decline exponentially with a correlation length of [8]

$$\xi_{\parallel} = \frac{L}{2\pi x}, \quad (2)$$

where x denotes the scaling dimension of the operator. Thus, one arrives at a FSS relation including the amplitude $A = 1/2\pi x$, implying universality of the correlation length itself.

Since there is an essential difference between the conformal groups in two dimensions, where it happens to be infinite dimensional, and higher dimensions, where it is reduced to a finite-dimensional Lie group, very few CFT results exceeding those already known from renormalisation-group arguments survive a transition to higher dimensions. However, considering the transformation (1) as a simple change of coordinates for a moment, rewriting it in polar coordinates allows for a generalisation to higher dimensions, now mapping \mathbb{R}^d to $S^{d-1} \times \mathbb{R}$. Noting that such a map only acts on the radial part of the coordinates, leaving the angular part invariant, Cardy [9] conjectured another linear amplitude-exponent relation for the correlation lengths in the geometry $S^{d-1} \times \mathbb{R}$, namely:

$$\xi_{\parallel} = \frac{R}{x}, \quad (3)$$

where R denotes the radius of S^{d-1} and $x = x(d)$ is again the scaling dimension. Note that this includes the $d = 2$ result (2) with $L = 2\pi R$. This relation, if it can be confirmed, constitutes one of the few exact results for non-trivial three-dimensional systems. Since the notion of primary of a scaling operator is *a priori* not well defined for $d > 2$, however, it is not entirely clear to which operators eq. (3) should apply. To find the analogues of primary operators for $d > 2$ one might start with the operator product expansion (OPE), cp. the explorative analysis of the operator content of the $O(n)$ models in three dimensions that can be found in ref. [10]. Note that this generalised mapping now connects *different* geometries, whereas the two-dimensional mapping can be understood as a meromorphism of the Riemann sphere onto itself.

Considering alternative approaches, attempts of numerical investigation of the FSS of systems on such spherical geometries are severely hampered by the fact that there is only a finite number of triangulations, *i.e.* regular polyhedra, for each sphere S^{d-1} . A numerical transfer matrix study for the case of $d = 3$ using Platonic solids as a regular discretisation of the sphere was found to be inconclusive due to the restriction in system sizes [11]. Here we follow a different line and use slightly irregular lattices as sphere discretisations for $d = 3$, exploiting and explicitly probing for the universality of the considered observables. Considering universality, it might be favourable to study *ratios* of correlation lengths which are known to be quite insensitive to lattice distortions. The attempt to escape such complications by considering the flat geometry $S^1 \times S^1 \times \dots \times \mathbb{R}$ instead surprisingly yields similar results, which are, however, up to now not connected to CFT calculations [12].

Lattice discretisation. – The most obvious model lattice with spherical topology is given by a cube covered by a rectangular mesh of lattice points, a lattice type that will be denoted

by (C) in the following. This inevitably introduces irregularities as compared to an idealized *regular* (large volume) triangulation of the sphere, which are given by a concentration of curvature around the cube corners and the defective coordination number of the corner points (three neighbours instead of four). In view of this problem several refinements have been proposed such as the replacement of the cube corners by triangular plaquettes, a construction that hides the coordination number defects away into the dual lattice, or the projection of the cube geometry (C) on the sphere S^2 by the application of appropriate weight factors to the links between lattice sites (S) [13]. This latter lattice can be shown to arrive at the “right” continuum field theory in the thermodynamic limit [14]. On the other hand, even simpler approximations could be devised such as for example a “pillow” resulting from the glueing together of rectangles along their four sides. Since, at least for bulk quantities, differences between those different choices of model lattices appear to be small [13], especially between (C) and its projected version (S), we here concentrate on the cubic discretisation (C) which is computationally much more convenient than (S). As far as universality is concerned, the *ratios* of asymptotic correlation lengths are found universal even with respect to marginal perturbations [15], so that we do not expect to see artefacts of discretisation defects here. Amplitude universality, however, might be sensitive to such distortions. Other types of lattice discretisations will be considered in a forthcoming publication [16].

The cube geometry (C) is being realised by six $L \times L$ square lattices appropriately glued together along their edges. Since the model lattices including type (C) are only topologically equivalent to spheres one has to conceive a definition of effective radii to enable a proper FSS analysis in the sense of eq. (3). Assigning a unit volume to each lattice site, to each pair of bonds, or to each individual square of the model lattice, respectively, on counting these entities one arrives at areas of

$$A = \begin{cases} 6L(L-2) + 8 & \text{“sites”,} \\ 6L(L-2) + 6 & \text{“bonds”, “squares”,} \end{cases} \quad (4)$$

from which the effective radii result via the relation $R = \sqrt{A/4\pi}$. Since for a “quadrangulation” one obviously has

$$4\#(\text{squares}) = 2\#(\text{bonds}), \quad (5)$$

the “bonds” and “squares” definitions coincide, but differ from the “sites” definition by a constant shift, leading to a slightly different approach to the leading FSS behaviour.

Model and simulation. – We consider a classical, ferromagnetic, nearest-neighbour Ising model with Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma_i = \pm 1. \quad (6)$$

The spins reside on lattices compound of the cubical sphere discretisation (C) with edge lengths L times a further linear lattice direction of length L_z . We apply periodic boundary conditions in z -direction to eliminate surface effects in modelling the infinite \mathbb{R} part. To control the effect of finite L_z still present we enforce the condition $L_z/\xi_{\parallel} \gg 1$ in a systematic way, *i.e.* we scale L_z proportionally to the radii R and thus (to leading order) proportionally to L . We use a ratio of $L_z/\xi_{\parallel} \approx 15$ which empirically proves sufficient to let the effect of finite L_z drop far below the threshold of statistical fluctuations. Simulations were done at a quite precise recent estimate for the Ising model critical coupling in three dimensions [17], $\beta_c = 0.221\,654\,4(3)$; the effect of critical coupling uncertainty was checked by a temperature reweighting technique and found negligible compared to statistical errors. For the FSS analysis we performed single-cluster

Monte Carlo simulations of nine systems with cube edge lengths ranging from $L = 4$ to $L = 12$, corresponding to effective radii of $R \approx 2$ to $R \approx 8$, and collected up to about $8 \cdot 10^6$ approximately independent measurements after an initial equilibration phase. Taking the scaled longitudinal sizes L_z into account, system sizes thus range up to about $3 \cdot 10^5$ spins.

Within the framework of CFT, the densities of magnetisation and energy turn out to be primary operators of spin models in two dimensions. Taking this as a hint for higher dimensions, we thus determine the longitudinal correlation lengths of these two observables to check whether Cardy's conjecture eq. (3) holds in the discretised case. We start measuring the corresponding connected, longitudinal correlation functions $G_{\sigma/\epsilon}^{c,\parallel}(z)$, maximally enhancing the statistics by appropriate averaging and projection techniques, for details see [18]. We find that for the extraction of the correlation lengths from this information at a level of high precision the customary way of fitting the correlation function data to the functional form $G(z)^{c,\parallel} = a \exp(-z/\xi_{\parallel}) + b$ for large distances z has severe drawbacks. Due to the statistical nature of the data one is not allowed to assume $b = 0$, *i.e.* the theoretical limit for infinite-length time series, *a priori* for finite-length measurements and is thus forced to use intrinsically unstable non-linear fits. Therefore, we resort to a difference-ratio type estimator of the form

$$\hat{\xi}_{\parallel}(z) = \Delta \left[\ln \frac{G^{c,\parallel}(z) - G^{c,\parallel}(z - \Delta)}{G^{c,\parallel}(z + \Delta) - G^{c,\parallel}(z)} \right]^{-1}, \quad (7)$$

which eliminates the inconvenient constants a and b above. The parameter $\Delta \geq 1$ controls the signal-noise ratio of the estimator and is being adapted for a minimum statistical error. To find final estimates for the correlation lengths $\xi_{\parallel}(R)$ of each system, we average the estimates $\hat{\xi}_{\parallel}(z)$ over a regime of distances z delimited by short distance deviations from the purely exponential behaviour and exploding fluctuations in the limit of very large distances. The averaging is done in a statistically optimized way entailing an expensive analysis of variances and covariances as well as autocorrelations, based on the ‘‘jackknife’’ resampling technique [18].

Results. – Collecting the final estimates for the correlation lengths $\xi_{\parallel,\sigma/\epsilon}$ of the densities of magnetisation and energy we arrive at the finite-size results shown in fig. 1(a), which scale linearly to leading order in the effective radii R defined above. Differences between the two radii definitions can hardly be distinguished at this scale. Plotting the effective amplitudes ξ_{\parallel}/R , however, reveals the presence of corrections to the leading scaling behaviour that are clearly resolvable at the given level of accuracy, cp. fig. 1(b). We thus fit our data to a FSS ansatz including a leading correction term,

$$\xi_{\parallel}(R) = AR + BR^{\alpha}, \quad (8)$$

treating α as an additional fit parameter that thus constitutes an *effective* correction exponent including parts of the higher-order corrections as well. This higher-order effect is kept small by successively removing points from the small R end while monitoring the quality-of-fit parameter Q . The range of points used is indicated by the range of the fit lines in fig. 1. Combining the fits to the data for the two different radii definitions we arrive at final estimates for the leading correlation length scaling amplitudes and their ratio of

$$\begin{aligned} A_{\sigma} &= 1.996(20), \\ A_{\epsilon} &= 0.710(38), \\ A_{\sigma}/A_{\epsilon} &= 2.81(15). \end{aligned} \quad (9)$$

Using weighted averages of recent estimates for the critical exponents of the three-dimensional Ising model [18], namely $\nu = 0.63005(18)$ and $\gamma = 1.23717(28)$, the conjectured amplitudes for

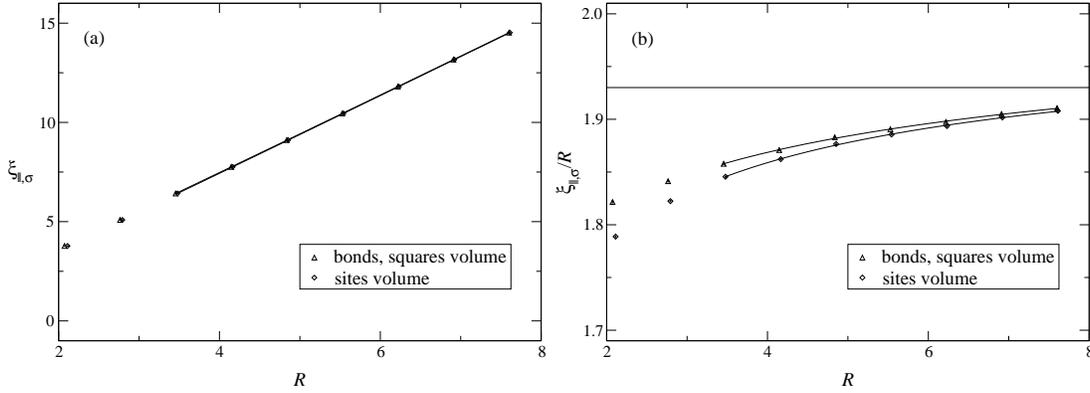


Fig. 1. – (a) FSS plot for the spin-spin correlation length $\xi_{||,\sigma}(R)$. (b) Scaling of the amplitudes $\xi_{||,\sigma}/R$. The continuous lines show fits described in the text and the horizontal line indicates the conjectured amplitude $A_\sigma^{\text{conj}} = 1.9298(13)$.

comparison are

$$\begin{aligned} A_\sigma^{\text{conj}} &= 1/x_\sigma = 2/(d - \gamma/\nu) = 1.9298(13), \\ A_\epsilon^{\text{conj}} &= 1/x_\epsilon = 1/(d - 1/\nu) = 0.70780(23), \\ A_\sigma^{\text{conj}}/A_\epsilon^{\text{conj}} &= x_\epsilon/x_\sigma = 2.7264(13), \end{aligned} \quad (10)$$

where $d = 3$ is understood, cp. eq. (3). Comparing the amplitude *ratios*, which are known to be more robust with respect to lattice inhomogeneities [15, 18], we find very good agreement between the simulation and Cardy’s conjecture. The same holds true for the amplitude of the energy-energy correlation length whose estimate is naturally less precise than that of the spin-spin correlation length. For the latter we still obtain reasonable agreement, but with a deviation of the numerical estimate towards larger values which is on the edge of statistical significance. To check whether this result indicates a systematic deviation due to the irregularity of the used lattice discretisation (C), simulations for the other discretisations mentioned above in the introduction should be performed [16].

Conclusions. – Approximating the sphere S^2 by a cube covered by a rectangular mesh of lattice points, we find that Cardy’s conjecture of a linear amplitude-exponent relation in the FSS of correlation lengths on the sphere-like geometry $S^{d-1} \times \mathbb{R}$ holds true for the case of the three-dimensional Ising model and the densities of magnetisation and energy. In terms of the analogy to CFT in two dimensions the considered operators are thus analogues of “primary” operators in three dimensions. The ratio of leading scaling amplitudes does, at the given level of accuracy, not show any effect of the irregularity of lattice discretisation; for the amplitude of the spin-spin correlation length further simulations using different discretisation schemes are necessary to judge the extent of universality that is being obeyed. Our results indicate that the geometry $S^2 \times \mathbb{R}$ considered here is closer to the original cylinder $S^1 \times \mathbb{R}$ (as far as the prevalence of universal features of correlation lengths scaling is concerned) than the toroidal geometry $T^2 \times \mathbb{R}$ which is not conformally flat, but nevertheless exhibits a scaling law quite similar to that found in two dimensions [12, 18].

MW gratefully acknowledges support by the “Deutsche Forschungsgemeinschaft” through the Graduiertenkolleg “Quantenfeldtheorie”.

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