Conformal Invariance of the Ising Model in Three Dimensions

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We investigate a critical Ising-like model in the curved geometry $S^2 \times \mathbb{R}^1$ obtained by a conformal mapping of the infinite 3D space $\mathbb{R}^3$. The incompatibility of regular lattices with this geometry is avoided by use of the anisotropic limit of the lattice Ising model, which renders one of the space coordinates continuous. We determine magnetic and energylike correlation lengths of this model by means of a cluster Monte Carlo algorithm. From these data, and the assumption of conformal invariance, we obtain the magnetic and temperature scaling dimensions as $X_h = 0.5178(12)$ and $X_t = 1.423(19)$, respectively. These numbers are in a good agreement with the existing results for the 3D Ising universality class.

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There exists a well-known relation between scaling dimensions of critical systems in two dimensions, and correlation lengths in a cylindrical geometry [1–5]. An adequate explanation was given by Cardy [6,7] on the basis of the assumption of conformal invariance, and a mapping of the two-dimensional space $\mathbb{R}^2$ on a cylinder $S^1 \times \mathbb{R}^1$. This relation is very useful because it provides a simple and powerful tool to determine scaling dimensions, and thus critical exponents, in two-dimensional models. For a model with scaling dimension X, the relation is [7]

$$\xi_R = R/X, \tag{1}$$

where ξ_R is the correlation length of a cylinder with radius R.

A similar relation exists in three dimensions [8]. In spherical coordinates, the line element in a flat space is

$$ds^2 = dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2). \tag{2}$$

Under the coordinate transformation

$$(r, \theta, \varphi) = (e^{u/R}, \theta, \varphi). \tag{3}$$

where $-\infty < u < \infty$, the line element transforms as

$$ds^2 = R^{-2} e^{2u/R}[du^2 + R^2(d\theta^2 + \sin^2\theta d\varphi^2)], \tag{4}$$

which can be recognized in terms of a scalar, position-dependent prefactor multiplying the natural metric,

$$ds^2 = du^2 + R^2(d\theta^2 + \sin^2\theta d\varphi^2), \tag{5}$$

of the curved space $S^2 \times \mathbb{R}^1$, i.e., a geometry which extends the surface S^2 of a sphere with radius R into another dimension $\mathbb{R}^1$. We shall refer to it as a "spherocylinder." The transformation (3) is thus conformal in combination with the metric (5). It relates models defined on $\mathbb{R}^3$ and on $S^2 \times \mathbb{R}^1$ as shown by Cardy [8].

Under the transformation (3), correlations of a scaling operator σ in a conformally invariant model behave covariantly as

$$\langle \sigma(u_1, \theta, \varphi)\sigma(u_2, \theta, \varphi)\rangle_{S^2\times\mathbb{R}^1} = R^{-2X} e^{X(u_1+u_2)/R} \langle \sigma(r_1, \theta, \varphi)\sigma(r_2, \theta, \varphi)\rangle_{\mathbb{R}^3}, \tag{6}$$

or, since $\langle \sigma(r_1, \theta, \varphi)\sigma(r_2, \theta, \varphi)\rangle \propto |r_1 - r_2|^{-2X}$,

$$\langle \sigma(u_1, \theta, \varphi)\sigma(u_2, \theta, \varphi)\rangle_{S^2\times\mathbb{R}^1} \propto R^{-2X} e^{-X|u_1-u_2|/R}(1 - e^{-|u_1-u_2|/R})^{-2X}. \tag{7}$$

For $|u_1 - u_2| \gg 0$, Eq. (7) decays exponentially,

$$\langle \sigma(u_1, \theta, \varphi)\sigma(u_2, \theta, \varphi)\rangle \propto R^{-2X} e^{-X|u_1-u_2|/R}, \tag{8}$$

so that relationship (1) follows again. In three dimensions, Eq. (8) was verified analytically for the special case of the spherical model [8]. A serious obstacle for numerical tests is that the curved space of Eq. (5) does not readily accommodate a sequence of regular lattices. Janke and Weigel [9] replaced the S^2 sphere by the surface of a cube. Their results for Ising models with finite size R satisfy Eq. (1) up to some proportionality constant. Remarkably, numerical investigations of systems in a flat, periodic $S^1 \times S^1 \times \mathbb{R}^1$ geometry with antiperiodic boundary conditions lead to similar results [10]. An explanation has not been given.

In this paper, we tackle the problem of simulations in a $S^2 \times \mathbb{R}^1$ geometry using the Hamiltonian limit of the lattice Ising model, which renders one of the coordinates continuous. We start from the Ising Hamiltonian in the 3D, flat space $\mathbb{R}^3$

$$\mathcal{H}/k_BT = -\sum_{x,y,z} [K_{xy} s_{x,y,z}(s_{x+1,y,z} + s_{x,y+1,z}) + K_z s_{x,y,z} s_{x,y,z+1}], \tag{9}$$

and take the anisotropic limit $\epsilon \to 0$ in

$$K_{xy} = \epsilon/t, \qquad e^{-2K_z} = \epsilon. \tag{10}$$

A Wolff-like cluster Monte Carlo method [11] is available for the system in this limit, which is equivalent with the

$d = 2$ quantum transverse Ising model. Since the correlation length, which determines the physical length scale, diverges as $1/\epsilon$ in the z direction, we choose the system size proportional to $1/\epsilon$ in that direction. Although the number of spins is thus divergent, it could be arranged such that the computer time remains finite. Simulations of the 3D model, combined with a finite-size-scaling analysis, yielded the critical point as $t = 3.0444(1)$ [11]. The precision achieved by this algorithm is good in comparison with other methods [12–14].

The divergence of the physical length scale in the z direction for $\epsilon \rightarrow 0$ suggests the use of a new coordinate $\tilde{z} \equiv \epsilon z/a$ in order to restore isotropy asymptotically. We have determined a by Monte Carlo simulations [15] as $a = 0.8881(2)$ from the requirement that the critical correlation functions of systems with periodic boundaries and sizes $(x, y, \tilde{z}) = (L, L, L)$ approach isotropy. Since the strong-coupling direction $\tilde{z}$ has become continuous, while x and y remain discrete, the 3D lattice reduces to an $L \times L$ system of lines. The weak couplings in the x and y directions connect to neighboring lines, and have a strength of a/t per unit of length as measured by $\tilde{z}$.

Because of its continuity in the $\tilde{z}$ direction, this model can be simulated in the curved $S^2 \times S^1$ geometry as follows. L evenly spaced circles on the S^2 sphere (see Fig. 1) serve as the loci of the spins, and define the strong-coupling direction $\tilde{z}$. Thus $L = \pi R$: The circumference of the sphere is 2 times the finite-size parameter L; that of S^1 is nL. We take n large enough in order to approximate the $S^2 \times \mathbb{R}^1$ geometry. We parametrize S^1 by $u = x = 1, 2, \ldots, nL$, and S^2 by θ and φ, with $\theta = \pi(y - \frac{1}{2})/L$, where $y = 1, 2, \ldots, L$, and $\varphi = \pi\tilde{z}/(L \sin\theta)$, where $0 \leq \tilde{z} < 2L \sin\theta$.

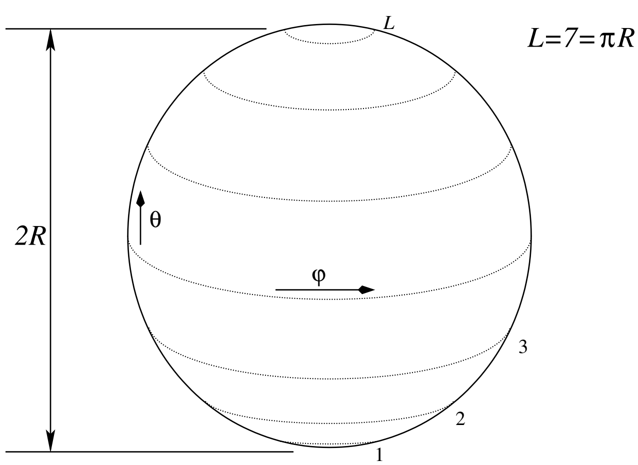

FIG. 1. Example of an S^2 sphere with finite size $L = 7$. It is a cross section of the $S^2 \times S^1$ geometry as used in the simulations. The circles represent continuous lines of spins in the strong-coupling direction. Weak couplings occur between adjacent circles within spheres as well as between those adjacent in the third dimension (the u direction, not shown).

At a given φ, the variables x and y form what is essentially a square lattice. The S^2 curvature is accounted for by the θ dependence of the period of $\tilde{z}$. The definition of the weak couplings between two points $[u, \varphi, \theta_\pm = \pi(y \pm \frac{1}{2})/L]$ still requires a length scale in the $\tilde{z}$ direction. To reduce discretization errors, we use the average length scale of both circles, i.e., $d\tilde{z} = d\varphi L(\sin\theta_+ + \sin\theta_-)/2\pi$.

We have simulated the above model on some 30 personal computers, for a total time of about 50 processor-months at 750 MHz. For system sizes $L = 4, 6, 8, 10, 12, 14, 16$ and $n = 4, 8$, we sampled the magnetic correlation function $g_m(r)$ in the u direction, defined as

$$g_m(r) = \frac{1}{V}\left\langle \sum_{u,\theta} \int_0^{2\pi} d\varphi \, \frac{L}{\pi} \sin\theta m(u, \theta, \varphi) \times m(u + r, \theta, \varphi) \right\rangle, \qquad (11)$$

where $m(u, \theta, \varphi)$ is the magnetization density at position φ, θ on the uth sphere, and $V = \sum_{u,\theta} 2L \sin\theta$ is the volume of the spherocylinder. We restrict $r \leq nL/2$ because of the periodic boundary.

We also sampled the interaction energy between adjacent circles, and its correlations in the u direction. We define e_{nn} as

$$e_{nn} = \frac{1}{V}\left\langle \sum_{u,\theta} \int_0^{2\pi} d\varphi \, \frac{L}{\pi} \sin\theta m(u, \theta, \varphi) \times m(u + 1, \theta, \varphi) \right\rangle, \qquad (12)$$

and the correlation function $g_e(r)$ as

$$g_e(r) = \frac{1}{V}\left\langle \sum_{u,\theta} \int_0^{2\pi} d\varphi \, \frac{L}{\pi} \sin\theta m(u, \theta, \varphi) \times m(u + 1, \theta, \varphi) m(u + r, \theta, \varphi) \times m(u + r + 1, \theta, \varphi) \right\rangle - e_{nn}^2 . \qquad (13)$$

For finite L, the critical singularities are rounded off, even on an infinitely long spherocylinder, because of the quasi-one-dimensional nature of the system. According to finite-size scaling, the singular part of the free energy density f behaves as

$$f(t, h, v, \ldots; L) = L^{-3} f(tL^{y_t}, hL^{y_h}, vL^{y_i}, \ldots; 1), \qquad (14)$$

where t is the temperaturelike scaling field, h is the magnetic field, v is the irrelevant field, and y_t, y_h, and y_i are the corresponding exponents. The corrections to scaling due to v are important only for small L because $y_i < 0$. The approximation of the sphere by L strips induces similar finite-size corrections. In analogy with errors due to the trapezium rule, we expect an effect on the mean temperature field of order L^{-2}, and corrections of order L^{y_c} with $y_c = y_t - 2$. These are likely to dominate over those

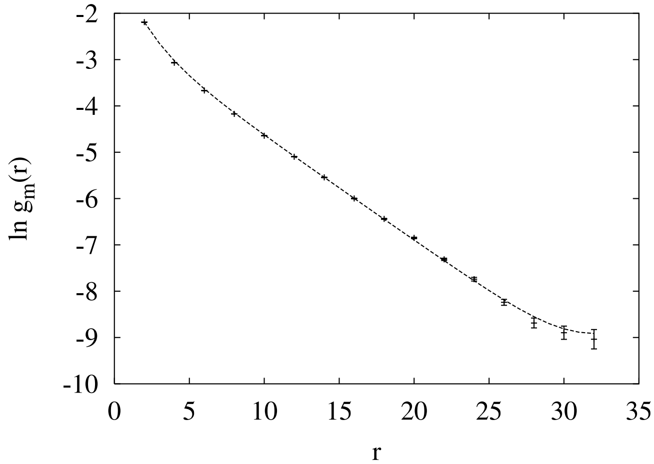

FIG. 2. Exponential decay of the magnetic correlation function $g_m(r, \frac{1}{L})$, shown as $\log g_m(r, \frac{1}{L})$ versus distance r. The system sizes are $L = 8$ and $nL = 64$. Error bars show the statistical uncertainty. A fit including corrections with amplitudes c_{m1} and c_{m2} is shown as the dashed line.

due to the irrelevant field, because $y_c \approx -0.413$ while $y_i \approx -0.815$ [15–18]. The irrelevant field modifies the correlation length ξ_L as [6]

$$\xi_L^{-1} = \frac{\pi X}{L}[1 + b_i L^{y_i} + \ldots]. \tag{15}$$

Our aim is to determine the scaling dimensions X via Eq. (1), i.e., from the exponential decay of $g(r, 1/L)$. Expansion of Eq. (7) for large $r = |u_1 - u_2|$ leads to

$$g\left(r, \frac{1}{L}\right) \propto L^{-2X} e^{-\pi X r/L} \left\langle 1 + \sum_j c_j e^{-j\pi r/L} \right\rangle, \tag{16}$$

where $c_j = \Gamma(2X + j)/\{\Gamma(2X - 1)\Gamma(j + 1)\}$.

Because of the periodicity of u, correlations build up over two distances r and $nL - r$. This effect, and corrections with an exponent y_c, lead to

$$g_m\left(r, \frac{1}{L}\right) = L^{-2X_h}\left[Y_1^{X_h(1+b_m L^{y_c})}\left(1 + \sum_j c_{mj} Y_1^j\right) + Y_2^{X_h(1+b_m L^{y_c})}\left(1 + \sum_j c_{mj} Y_2^j\right)\right](A_m + v_m L^{y_c}), \tag{17}$$

and

$$g_e\left(r, \frac{1}{L}\right) = L^{-2X_h}\left[Y_1^{X_h(1+b_e L^{y_c})}\left(1 + \sum_j c_{ej} Y_1^j\right) + Y_2^{X_h(1+b_e L^{y_c})}\left(1 + \sum_j c_{ej} Y_2^j\right)\right](A_e + v_{e1} L^{y_c}) + v_{e2} L^{y_1}, \tag{18}$$

where $Y_1 = e^{-\pi r/L}$, $Y_2 = e^{-\pi(n - r/L)}$, and $y_1 = 4y_t - 2d - 2 \simeq -1.652(4)$. The correction with amplitude v_{e2} is due to the inhomogeneity of the energy caused by the approximation of the sphere [15].

The Monte Carlo data are well fitted by these formulas, according to the χ^2 criterion. Examples are shown in Figs. 2 and 3. The upward trends on the right are due to the periodic boundary.

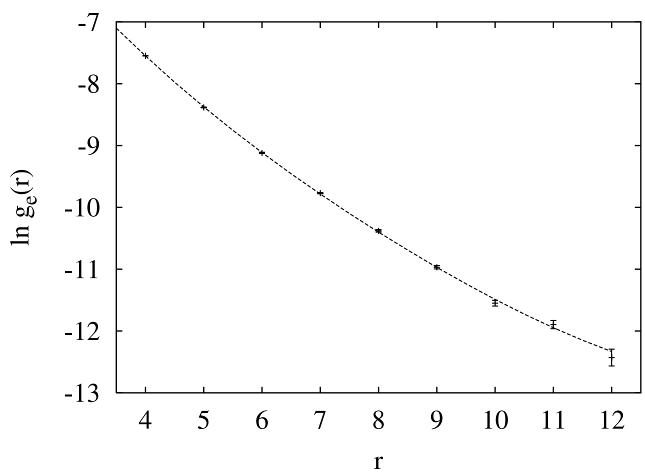

FIG. 3. Exponential decay of the energy-energy correlation function $g_e(r, \frac{1}{L})$, shown as $\log g_e(r, \frac{1}{L})$ versus distance r (horizontal). The system sizes are $L = 8$ and $nL = 32$. Error bars show the statistical uncertainty. The dashed line shows a fit with correction amplitudes c_{e1}, c_{e2}, c_{e3}, v_{e1}, and v_{e2}.

The exponent $-2X_h$ of L was fixed at $2y_h - 6 = -1.0370(6)$ [15–18], and $y_c = -0.413$ as explained above. The c_{mj} are found by substituting $2X_h = 1.037(10)$ in Eq. (16). The fitted parameters are shown in Table I. The quality of the fits indicates that the length ratio $n = 4$ already yields a reasonable approximation of infinitely long systems. The result $X_h = 0.5195(24)$ is already close to the expected value $3 - y_h = 0.5185(3)$ [15,16]. An even better fit is obtained for systems whose long size is $8L$. Then, the χ^2 criterion allows a cutoff at

TABLE I. Results of three least-squares fits to $g_m(r, \frac{1}{L})$, each using a different combination of unknown parameters.

n	4 Fit1	8 Fit2	8 Fit3
$L_{\min}$	10	8	8
$L_{\max}$	16	16	16
$(r/L)_{\min}$	1.2	1.0	1.0
$(r/L)_{\max}$	4.0	4.0	4.0
X_h	0.5195 (24)	0.5178 (12)	0.5178 (12)
A_m	0.7562 (88)	0.7438 (10)	0.7440 (14)
b_m	0.1056 (48)	0.1084 (30)	0.1086 (30)
v_m	...	...	0.000 01 (8)

TABLE II. Simulation lengths in millions of samples of the quantities $g_m(r, \frac{1}{L})$ and $g_e(r, \frac{1}{L})$, respectively. Samples were taken at intervals of five Wolff clusters.

	$g_m(r, \frac{1}{L})$		$g_e(r, \frac{1}{L})$
L/n	4	8	4
4	341	73	...
6	511	73	24 838
8	682	243	73 064
10	1096	487	114 045
12	1023	1242	12 296
14	1278	937	...
16	487	1656	...

TABLE III. Least-squares fit of $g_e(r, \frac{1}{L})$, for systems with size ratio $n = 4$.

$L_{\min}$	$L_{\max}$	$(r/L)_{\min}$	$(r/L)_{\max}$	X_t
8	12	0.60	1.5	1.423(19)
A_e	b_e	v_{e2}	v_{e1}	...
0.788(23)	...	0.0160(55)	−0.0053(14)	...

even smaller system sizes $L_{\min}$ and distances $(r/L)_{\min}$, and the result $X_h = 0.5178(12)$ is again close to the expected value.

Since the energy-energy correlation decays relatively fast, it is more difficult to determine X_t. Thus much longer simulations were needed for this purpose (see Table II). We obtain $X_t = 1.423(19)$ (see Table III), which agrees well with the expected value $X_t = 1.413(1)$ [15,16]. Although the parameter v_{e2} is quite small, it is necessary to obtain an acceptable residual χ^2. The rapid decay of the correlation functions did not allow the resolution of a correction with amplitude b_e. Several modifications of the fit formula were tried, for instance, including corrections with an irrelevant exponent y_i, but these did not lead to significant reductions of the residual χ^2.

In conclusion, we have confirmed the covariant behavior of the magnetic and energylike correlation functions under a conformal transformation in three dimensions, and shown that it is possible to determine the critical scaling dimensions from the correlation lengths of finite systems in an appropriate geometry.

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