Anisotropic Scaling and Generalized Conformal Invariance at Lifshitz Points

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(Received 21 March 2001; published 31 August 2001)

The behaviour of the 3D axial next-nearest-neighbor Ising model at the uniaxial Lifshitz point is studied using Monte Carlo techniques. A new variant of the Wolff cluster algorithm permits the analysis of systems far larger than in previous studies. The Lifshitz point critical exponents are $\alpha = 0.18(2)$, $\beta = 0.238(5)$, and $\gamma = 1.36(3)$. Data for the spin-spin correlation function are shown to be consistent with the explicit scaling function derived from the assumption of local scale invariance, which is a generalization of conformal invariance to the anisotropic scaling *at* the Lifshitz point.

DOI: 10.1103/PhysRevLett.87.125702 PACS numbers: 64.60.–i, 05.70.Jk, 64.70.Rh, 11.25.Hf

The modern understanding of critical phenomena is governed by the notion of scale invariance [1]. For isotropic critical systems the extension from global, spatially homogeneous scaling to space-dependent rescaling factors leads to the requirement of conformal invariance of the correlators. This approach has proven to be very fruitful when examining isotropic equilibrium critical systems, especially in two dimensions [1–3].

On the other hand, little is known for systems with strongly anisotropic critical points, where the value of the anisotropy exponent θ differs from unity. In these cases, the two-point function $C(\vec{r}_\perp, r_\parallel)$ satisfies the scaling form

$$C(\vec{r}_\perp, r_\parallel) = b^{-2x} C(b\vec{r}_\perp, b^\theta r_\parallel) = r_\perp^{-2x} \Omega(r_\parallel r_\perp^{-\theta}), \quad (1)$$

where $r_\parallel$ and $r_\perp = |\vec{r}_\perp|$ are the distances parallel and perpendicular with respect to a chosen axis, x is a scaling dimension, θ is the anisotropy exponent, and $\Omega(v)$ is a scaling function. Scale invariance alone is not enough to determine the form of the function $\Omega(v)$.

Recently, a generalization of conformal invariance involving local space-time-dependent scale transformations for anisotropy exponents $\theta \neq 1$ has been proposed [4]. This approach attempts to generalize the scaling (1), usually considered with b constant, to space-dependent rescaling $b = b(\vec{r}_\perp, r_\parallel)$, thereby assuming that the two-point functions still transform in a simple way. These transformations are constructed, starting from the conformal transformations $r_\parallel \to (\alpha r_\parallel + \beta)/(\gamma r_\parallel + \delta)$ with $\alpha\delta - \beta\gamma = 1$, in such a way that the transformations in the "spatial" coordinates $\vec{r}_\perp$ are consistent with the anisotropic scaling (1). Systems which are invariant under these transformations and whose correlators, generalizing (1), transform covariantly under them are said to satisfy *local scale invariance* (LSI). It turns out that if $\theta = 2/N$, where N is a positive integer, $\Omega(v)$ satisfies the differential equation [4]

$$\alpha_1 \frac{d^{N-1}\Omega(v)}{dv^{N-1}} - v^2 \frac{d\Omega(v)}{dv} - \zeta v \Omega(v) = 0, \quad (2)$$

where $\zeta = 2x/\theta$ and α_1 is a constant. Equation (2) can be explicitly solved [4] in terms of hypergeometric functions ${}_2F_{N-1}$ (conformal invariance is reproduced [4] for $N = 2$, and $N = 1$ gives the nonrelativistic Schrödinger invariance [5]). Evidently, the above hypothesis of LSI in systems satisfying (1) is a strong one and relies on certain assumptions about the structure of the underlying field theory (FT). We shall test the idea of LSI by checking the resulting expressions for $\Omega(v)$ in a nontrivial spin system which satisfies the strongly anisotropic scaling (1) [6].

While dynamical scaling (1) occurs in critical dynamics (then θ is referred to as dynamical exponent) or in true nonequilibrium phase transitions such as directed percolation, well-known examples of stongly anisotropic *equilibrium* criticality are the *Lifshitz points* [7] encountered in systems with competing interactions. At a Lifshitz point, a disordered, a uniformly ordered, and a periodically ordered phase become indistinguishable [7]. The simplest model for these is the ANNNI (axial next-nearest-neighbor Ising) model [8] which describes faithfully, among others, magnetic systems, alloys, or uniaxially modulated ferroelectrics [9–11]. Recently, a large variety of new physical systems (ferroelectric liquid crystals [12], uniaxial ferrolectrics [13], block copolymers [14], or even quantum systems [15]) were shown to possess a Lifshitz point which has stimulated renewed interest in its properties. Furthermore, new field theory studies [16–19] have led to more refined estimates (in the framework of an ϵ expansion) of the critical exponents of the general m-fold Lifshitz points in d dimensions with a n-component order parameter [16–18].

We study the 3D ANNNI model on a cubic lattice with periodic boundary conditions. The Hamiltonian is

$$\mathcal{H} = -J \sum_{xyz} s_{xyz}(s_{(x+1)yz} + s_{x(y+1)z} + s_{xy(z+1)}) + \kappa J \sum_{xyz} s_{xyz} s_{xy(z+2)}, \quad (3)$$

with $s_{xyz} = \pm 1$, whereas $J > 0$ and $\kappa > 0$ are coupling constants. In the z direction, competition between ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor couplings takes place, leading to a

rich phase diagram with a multitude of different phases, both commensurate and incommensurate to the underlying cubic lattice [8]. The anisotropy exponent $\theta = \nu_\parallel/\nu_\perp$, where $\nu_\parallel$ und $\nu_\perp$ are the exponents of the correlation lengths parallel and perpendicular to the z axis. At the uniaxial Lifshitz point, a recent careful field-theoretical calculation [17] showed that $\theta = \frac{1}{2} - a\epsilon^2 + O(\epsilon^3)$ in a second-order ϵ expansion (with $\epsilon = 4.5 - d$), where $a \simeq 0.0054$ for the 3D ANNNI model.

Our main purpose will be the numerical computation and thorough analysis of the critical spin-spin correlation function *at* the uniaxial Lifshitz point of the ANNNI model through a large-scale Monte Carlo (MC) simulation. The agreement between our numerical results and the analytic expression for $\Omega(v)$ derived from (2) presents evidence that local scale invariance, as formulated in Ref. [4], is realized as a new symmetry in strongly anisotropic equilibrium critical systems.

Such a study does require reliable and precise estimates of the critical exponents. However, published estimates of critical exponents obtained with different techniques spread considerably; see Table I. We therefore undertook extensive Monte Carlo simulations to estimate the exponents reliably. Previous Monte Carlo studies [20] considered only small systems of (mostly) cubic shape. Here, we present calculations for large systems of anisotropic shape with $L \times L \times N$ spins, with $20 \leq L \leq 240$ and $10 \leq N \leq 100$, taking into account the special finite-size effects coming from the anisotropic scaling at the Lifshitz point [22]. This is the first study of the ANNNI model where the exponents α, β, and γ are computed independently.

As usual, the problems coming from critical slowing down, encountered when using local Monte Carlo dynamics, are alleviated by using nonlocal methods, such as the Wolff cluster algorithm [23]. For the Ising model with only a nearest-neighbor coupling J, this algorithm may be described as follows: one chooses randomly a lattice site, the seed, and then builds up iteratively a cluster by including a lattice site j (with spin s_j), neighbor to a cluster site i (with spin s_i), with probability $p = \frac{1}{2}[1 + \mathrm{sgn}(s_i s_j)]\{1 - \exp[-2J/(k_B T)]\}$. One ends up with a cluster of spins, all having the same sign, which is then flipped as a whole. These types of same-sign clusters are obviously not adapted to our problem because of the competing interactions along the z direction; see (3).

We therefore propose the following modified cluster algorithm. Starting with a randomly chosen seed, one again builds up iteratively a cluster. Consider a newly added cluster lattice site i with spin s_i. A lattice site j, with spin s_j nearest neighbor to i, is included with probability $p_n = p$, whereas an *axial* next-nearest-neighbor site k with spin s_k is included with probability $p_a = \frac{1}{2}[1 - \mathrm{sgn}(s_i s_k)]\{1 - \exp[-2J\kappa/(k_B T)]\}$. Thus, the final cluster, which will be flipped as a whole, contains spins of both signs. Ergodicity and detailed balance are proven as usual. This algorithm works extremely well in the ferromagnetic phase and in the vicinity of the Lifshitz point. Generalization to other systems with competing interactions is straightforward. For the computation of the spin-spin correlation function we adapt in a similar way a recently proposed very efficient algorithm using Wolff clusters [24]. This algorithm yields the infinite-system correlation functions at temperatures above T_c and greatly reduces finite-size effects at the critical temperature as compared to a more traditional approach.

We now outline the determination of the critical exponents. The results are listed in Table I. Usually, 4×10^4 clusters were generated per run, discarding the first 10^4 clusters for equilibration. We averaged over an ensemble of at least 15 runs using different random numbers to obtain the final thermal averages. As an example, Fig. 1 shows the effective exponent $\beta_{\mathrm{eff}} = d\ln m/d\ln t$, where m denotes the magnetization and $t = 1 - T/T_c$. In the limit $t \to 0$ the effective exponent yields the critical exponent [25] β, provided finite-size effects can be neglected. The two sets of data in Fig. 1 correspond to two different paths in the temperature-interaction space, both ending at the point ($\kappa = 0.270$, $T_c = 3.7475$), setting $J/k_B = 1$.

TABLE I. Critical exponents at the Lifshitz point of the 3D ANNNI model, as obtained from Monte Carlo simulations, high-temperature series expansion, and renormalized field theory. The numbers in parentheses give the estimated error in the last digit(s).

	α	β	γ	$(2-\alpha)/\gamma$	β/γ
MC[a]	⋯	0.19(2)	1.40(6)	⋯	0.14(2)
HT[b]	0.20(15)	⋯	1.6(1)	1.1(2)	⋯
FT[c]	⋯	⋯	⋯	1.27	0.134
FT[d]	0.160	0.220	1.399	1.315	0.157
MC	0.18(2)	0.238(5)	1.36(3)	1.34(5)	0.175(8)

[a]See Ref. [20]. [b]See Ref. [21]. [c]See Ref. [17]. [d]See Ref. [18].

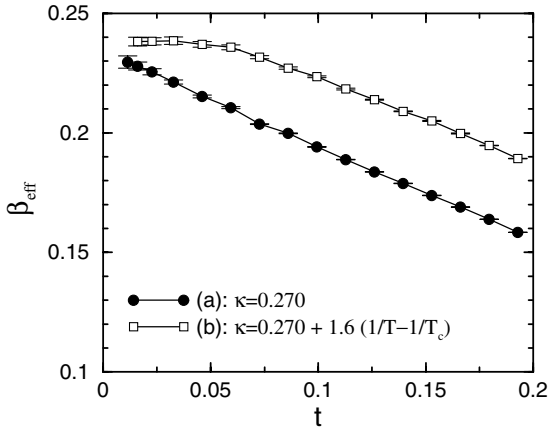

FIG. 1. Effective exponent β_{eff} versus t for two different trajectories in the (T, κ) space; see text. Error bars include the uncertainty in T_c: $T_c(\kappa = 0.270) = 3.7475 \pm 0.0005$.

For set (a), κ was fixed at 0.270, whereas, for set (b), $\kappa = 0.270 + 1.6(1/T - 1/T_c)$. The corrections to scaling for set (b) are small compared to set (a), resulting in a plateau for $t \leq 0.06$, thus making a very precise estimation of β possible. Of course, finite-size effects have to be monitored carefully. As usual, we adjust the system size in order to circumvent finite-size dependences [25]. For the determination of the susceptibility and specific heat critical exponents γ and α (see Table I), data obtained at temperatures both below and above T_c were analyzed. Our error bars take into account the sample averaging as well as the uncertainty in the location of the Lifshitz point. Based on our data, we locate the Lifshitz point at $\kappa = 0.270 \pm 0.004, T_c = 3.7475 \pm 0.0005$, thus confirming a high-temperature (HT) series estimate [26].

The agreement of the independently estimated exponents α, β, and γ with the scaling relation $\alpha + 2\beta + \gamma = 2$, up to $\approx 0.8\%$, illustrates the reliability of our data.

We are now ready to discuss the scaling of the spin-spin correlation function $C(\vec{r}_\perp, r_\parallel) = \langle s_{\vec{r}_\perp, r_\parallel} s_{\vec{0},0} \rangle$ and its scaling function $\Omega(v)$ as defined in (1). In $(d_\perp + 1)$ dimensions, one has $\zeta = 2(d_\perp + \theta)/\theta(2 + \gamma/\beta)$. For the 3D ANNNI model, $\zeta = 1.30 \pm 0.05$, where the error follows from the errors in the values of the critical exponents. In Fig. 2 we show selected data for the function

$$\Phi(u) = u^{-\zeta} \Omega(1/u), \tag{4}$$

with $u = \sqrt{r_\perp}/r_\parallel$, as computed by Monte Carlo simulations of a system with $200 \times 200 \times 100$ spins (assuming [27] $\theta = 1/2$). This permits a nice visual test of the data collapse and establishes scaling. Note that Fig. 2 was

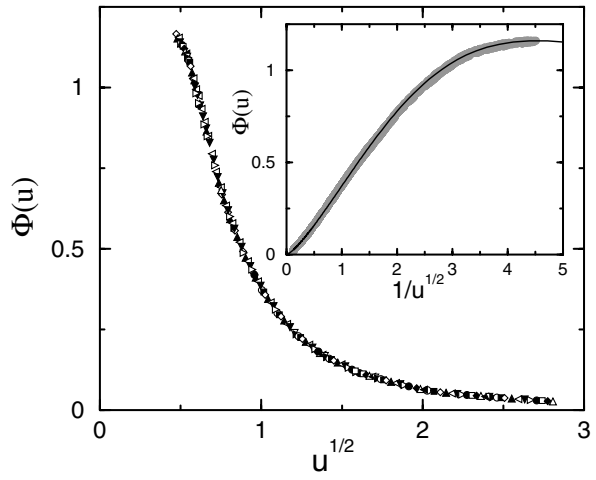

FIG. 2. Scaling funtion $\Phi(u)$ (see text) versus $u^{1/2} = (\sqrt{r_\perp}/r_\parallel)^{1/2}$ for $\kappa = 0.270$ and $T = 3.7475$. Selected Monte Carlo data for a system of $200 \times 200 \times 100$ spins are shown [27]. The different symbols correspond to 26 distinct values of $r_\perp$, with $2\sqrt{12} \leq r_\perp \leq 2\sqrt{46}$. Inset: comparison of the full data set of 1.7×10^4 points for the scaling function $\Phi(u)$ (gray points) with the analytical prediction Eq. (5) following from the assumption of LSI, with $p = -0.11$, $\alpha_1 = 33.2$, and $b_0 = 0.41$ (solid curve).

obtained after taking into account more than five million cluster updates.

The small deviations (of order $\approx 2\%$) from the value $\theta = 1/2$ obtained in recent field-theoretical calculations [17] are not yet distinguishable [27] from the purely numerical errors in our data and the exponents derived from them. Therefore, for our purposes, namely the test of LSI, it is enough to set $\theta = 2/N = 1/2$, leading to $N = 4$ in the differential equation (2) [6]. In addition, the scaling form (1) implies the boundary condition $\Omega(v) \sim v^{-\zeta}$ for $v \to \infty$. For $N = 4$, there are two independent solutions of Eq. (2) satisfying this boundary condition [3,4], and the scaling function becomes

$$\Omega(v) = b_0 F_0\big(v/(4\alpha_1)^{1/4}\big) + b_1 v F_1\big(v/(4\alpha_1)^{1/4}\big), \tag{5}$$

where $F_{0,1}$ are explicitly given in Eqs. (18) and (19) of Ref. [4]. Here α_1 is the constant occurring in (2) and $b_{0,1}$ are free parameters. Since b_0 and α_1 are merely scale factors, the functional form of the scaling functions $\Omega(v)$ and $\Phi(u)$ depends on the single *universal* parameter $p := \alpha_1^{1/4} b_1/b_0$.

To see this, consider the moments $M(n) := \int_0^\infty du\, u^n \Phi(u)$. For $\theta = 1/2$ and taking into account (5), it follows [28] that in the scaling region the moment ratios

$$J(\{m_i\};\{n_j\}) := \prod_{i=1}^{k} M(m_i) \Big/ \prod_{j=1}^{k} M(n_j), \tag{6}$$

with $k \geq 2$ and $\sum_i m_i = \sum_j n_j$, are independent of b_0 and α_1 and only depend on the functional form of $\Phi(u)$ as parametrized by p. Our Monte Carlo data for the spin-spin correlator will be consistent with LSI if the values of p determined from several different ratios J coincide.

Since we are not able to compute numerically the function $\Phi(u)$ for values of u below $u_0 \approx 0.22$, a direct analysis along the lines just sketched is not possible. Instead we have to consider the moments $\tilde{M}(n) := \int_{u_0}^\infty du\, u^n \Phi(u\alpha_1^{1/4}) = \alpha_1^{-(n+1)/4} \int_{w_0}^\infty dw\, w^n \Phi(w)$ with $w_0 = u_0 \alpha_1^{1/4}$. The moment ratios $\tilde{J}(\{m_i\};\{n_j\})$ [defined in complete analogy with (6)] then depend on the scale factor $\alpha_1^{1/4}$ through w_0. The parameters α_1 and p are determined from the following scheme. By choosing a suitable starting value for α_1 we compute an approximative value for p by comparing the values of the moment ratios $\tilde{J}$ [obtained from the full data set for $\Phi(u)$ as shown in the inset of Fig. 2] with the p-dependent expressions coming from integrating the $\tilde{M}(n)$ using the analytic form (5). An improved value for α_1 is then derived by comparing the values $\tilde{M}(m)/\tilde{M}(n)$ for arbitrary m and n obtained (i) from our numerical data and (ii) from the analytical expressions after inserting the value of p. The final values of α_1 are obtained by averaging over five different pairs (m, n).

The values of p and α_1 determined from several distinct moment ratios are collected in Table II. We obtain

TABLE II. Values of the parameters p and α_1 computed from different moment ratios $\tilde{J}(\{m_i\};\{n_j\})$; see text.

$\{m_i\}$	$\{n_j\}$	p	α_1
$\{0, -0.5\}$	$\{-0.25, -0.25\}$	-0.102	32.7
$\{-0.25, -0.75\}$	$\{-0.5, -0.5\}$	-0.125	34.0
$\{0.2, -0.9\}$	$\{0, -0.7\}$	-0.100	32.8
$\{0.2, -0.6, -0.8\}$	$\{-0.3, -0.4, -0.5\}$	-0.102	32.8
$\{-0.1, -0.6, -0.7\}$	$\{-0.4, -0.5, -0.5\}$	-0.117	33.5

the mean values $p = -0.11(1)$ and $\alpha_1 = 33.2(8)$. The consistency of the different determinations of the two parameters provides clear evidence in favor of the applicability of the hypothesis of local scale invariance to the Lifshitz point of the ANNNI model.

Finally, $b_0 \approx 0.41$ is obtained by adjusting the scale of Φ. Inserting these values into the analytical expression yields for Φ the solid curve shown in the inset of Fig. 2. The agreement between our MC data and the theoretical result is remarkable.

Local scale invariance was confirmed before at the Lifshitz point of the axial next-nearest-neighbor spherical (ANNNS) model. In that exactly solvable model, the Ising model spins in (3) are replaced by spherical model spins $s_{xyz} \in \mathbb{R}$ together with the usual spherical constraint [8]. At the Lifshitz point, one has $\theta = 1/2$ and the exactly known spin-spin correlator [29] agrees with the scaling form (5) for $b_1 = 0$ [4]. Our finding that LSI also appears to hold for the ANNNI model suggests that the domain of validity of LSI should extend beyond the context of free field theory which underlies the ANNNS model. It appears plausible that LSI will also hold true for the Lifshitz points of the axial next-nearest-neighbor XY (ANNNXY), axial next-nearest-neighbor Heisenberg (ANNNH), ... models [8] which are intermediate between the ANNNI and the ANNNS model. Since the number of dimensions $d_\perp$ merely enters as a parameter, local scale invariance could also be tested along the lines of an ϵ expansion [17].

In conclusion, the precise localization of the 3D ANNNI model Lifshitz point and improved estimates of its critical exponents allowed one, for the first time, to determine reliably the scaling of the spin-spin correlator. Its functional form was found to agree with the prediction of local scale invariance. The confirmation of the applicability of local scale invariance to this situation suggests a new symmetry principle for the description of equilibrium systems with anisotropic scaling, especially for systems with competing interactions at their Lifshitz points.

We thank H. W. Diehl and M. Shpot for communicating their two-loop results [18] before publication and the CINES Montpellier for providing substantial computer time (Project No. pmn2095). M. P. is supported by EU Contract No. HPMF-CT-1999-00375.

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