Analytical scale and Generalized Conformal Invariance at Tadpole Points
rich phase diagram with a multitude of different phases, both commensurate and incommensurate to the underlying cubic lattice. The anisotropy exponent \( \theta \equiv \nu_1/\nu_2 \), where \( \nu_1 \) and \( \nu_2 \) 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 shows that \( \theta = 4 - \epsilon \) in a second-order \( \epsilon \)-expansion (with \( \epsilon = 4.5 - d \)) where \( d \approx 0.0054 \) for the 3D ANNNI model.

Our main purpose will be the numerical computation and thorough analysis of the critical spin-spin correlation function of the uniaxial Lifshitz point of the ANNNI model through a large-scale Monte Carlo 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 large-scale Monte Carlo simulations to estimate the exponents reliably. Previous Monte Carlo studies 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 anisotropically scaling at the Lifshitz point. This is the first study of the ANNNI model where the exponents \( \alpha, \beta, \) and \( \gamma \) are computed independently.

As usual, the problems coming from critical slowing down encountered when using local Monte Carlo dynamics, are alleviated by using non-local methods, such as the Wolff cluster algorithm. For the Ising model with only a nearest neighbour 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 \( s_j \)), neighbour to a cluster site \( i \) (with spin \( s_i \)), with probability \( p = 1/2 (1 + \text{sign}(s_is_j)) / [1 + \exp \{-2J/(k_BT)\}] \). One ends up with a cluster of spins having all the same sign which is then flipped as a whole. This kind 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 neighbour to \( i \) is included with probability \( p_{in} = p \), whereas an axial next-nearest neighbour site \( k \) with spin \( s_k \) is included with probability \( p_{2n} = 1/2 (1 - \text{sign}(s_is_k)) / [1 + \exp \{-2J/(k_BT)\}] \). 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. This algorithm yields the infinite-system correlation functions at temperatures above \( T_c \) and largely reduces finite-size effects at the critical temperature as compared to a more traditional approach. These algorithms will be discussed in detail elsewhere.

We now outline the determination of the critical exponents. The results are listed in Table I. As an example, Figure 1 shows the effective exponent

\[
\beta_{\text{eff}} = \frac{d \ln m}{d \ln T},
\]

where \( m \) denotes the magnetization and \( T = 1 - \left( T/T_c \right) \).

In the limit \( T \to 0 \) the effective exponent yields the critical exponent \( \beta \), provided finite-size effects can be neglected. The two sets of data in Figure 1 correspond to two different paths in the temperature-interaction space, both ending at the point \( (\kappa = 0.270, T_c = 3.7475) \), setting \( J/k_B = 1 \). For set (a) \( \kappa \) was fixed at 0.270, whereas for set (b) \( \kappa = 0.270 + 0.1 (1/T - 1/T_c) \). 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 \( \beta \) 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.

For the determination of the susceptibility and specific heat critical exponents \( \gamma \) and \( \alpha \), see Table I, data obtained at temperatures both below and above \( T_c \) were analysed. 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 an estimation from a high temperature series expansion.

The agreement of the independently estimated exponents \( \alpha, \beta \) and \( \gamma \) 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 \( C(\mathbf{r}_1, \mathbf{r}_2) \equiv \langle s_{\mathbf{r}_1} s_{\mathbf{r}_2} \rangle \) and its scaling function \( \Omega(v) \) as defined in (1). In \((d_{\parallel} + 1)\) dimensions, one has \( \zeta = 2(d_{\parallel} + \theta)/[\theta(2 + \gamma/\beta)] \). 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 Figure 2 we show selected data for the function

\[
\Phi(u) = u^{-\zeta} \Omega(1/u)
\]

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

The small deviations (of order \( \approx 2\% \)) from the value \( \theta = 1/2 \) obtained in recent field-theoretical calculations are not yet distinguishable 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). In addition, the scaling form (4) implies the boundary condition \( \Omega(v) \sim v^{-k} \) for \( v \to \infty \). For \( N = 4 \), there are two independent solutions of eq. (2) satisfying this boundary condition \(^3\) and the scaling function becomes

\[
\Omega(v) = b_0 F_0(v/(4\alpha_1)^{1/4}) + b_1 v F_1(v/(4\alpha_1)^{1/4}) \quad (6)
\]

where \(^4\)

\[
F_0(x) = \frac{\Gamma(3/4)}{\Gamma(C/4)} \sum_{n=0}^{\infty} \frac{\Gamma(n/2 + \zeta/4)}{n!\Gamma(n/2 + 3/4)} (-x^2)^n 
\]

\[
F_1(x) = \frac{\Gamma(3/2)}{\Gamma(\frac{1}{4}C + 1)} \sum_{n=0}^{\infty} \frac{\Gamma((n + 1 + \zeta)/4) s(n)}{\Gamma(n/4 + 1) \Gamma(n/4 + 3/4)} (-x^n) 
\]

and \( s(n) = \frac{1}{\sqrt{\pi}} \left( \cos \frac{\zeta}{2} + \sin \frac{\zeta}{2} \cos \frac{\frac{n}{2}}{2} \right) \cos \frac{\frac{n}{2}}{2} \). Here \( \alpha_1 \) is the constant occurring in (2) and \( b_0, b_1 \) are free parameters. Since \( b_0 \) and \( \alpha_1 \) are merely scaling factors, the functional form of the scaling functions \( \Omega(v) \) and \( \Phi(u) = u^{-1} \Omega(1/u) \) depends on the single universal parameter

\[
p = \frac{\alpha_1}{b_1} \frac{1}{b_0} \quad (7)
\]

To see this, consider the moments \( M(n) := \int_0^\infty u^n \Phi(u) \). For \( \theta = 1/2 \) and taking into account (6), it follows \(^8\) that in the scaling region the moment ratios

\[
J(\{m_i\}; \{n_j\}) = \prod_{i=1}^{k} M(m_i) / \prod_{j=1}^{k} M(n_j) \quad (8)
\]

with \( k \geq 2 \) and \( m_i = \sum_{j} n_j \) are independent of \( b_0 \) and \( \alpha_1 \) and only depend on the functional form of \( \Phi(u) \) as parameterized 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.

As 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 \( \tilde{M}(n) := \int_0^{u_0} u^n \Phi(u) \Phi(u)^{1/4} = \alpha_1 1/4 \int_0^{u_0} u^n \Phi(u) \Phi(u)^{1/4} \) with \( u_0 = u_0 \alpha_1^{1/4} \). The moment ratios \( \tilde{J}(\{m_i\}; \{n_j\}) \) (defined in complete analogy with (8)) then depend on the scale factor \( \alpha_1^{1/4} \) through \( u_0 \). The parameters \( \alpha_1 \) and \( p \) are determined from the following scheme. Choosing a suitable starting value for \( \alpha_1 \) we compute an approximate 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 Figure 2) with the \( p \)-dependent expressions coming from integrating the \( M(n) \) using the analytic form (6, 7). An improved value for \( \alpha_1 \) is then derived by comparing the values \( M(m_i)/M(n_j) \) 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 \( \alpha_1 \) are obtained by averaging over five different pairs \( (m, n) \).

The values of \( p \) and \( \alpha_1 \) determined from several distinct moment ratios are collected in Table II. We obtain 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 favour 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 \( \Phi \). Inserting these values into the analytical expression yields for \( \Phi \) the full curve shown in the inset of Figure 2. The agreement between our MC data and the theoretical result is remarkable.

Local scale invariance had been confirmed \(^9\) before at the Lifshitz point of the ANNNI model. In that exactly solvable model, the Ising model spins in (3) are replaced by spherical model spins \( s_{xyz} \in \mathbb{R}^3 \) together with the usual spherical constraint. \(^7\) At the Lifshitz point, one has \( \theta = 1/2 \) and the exactly known spin-spin correlator \(^5\) agrees with the scaling form (6) 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 ANNNI model. It appears plausible that LSI will also hold true for the Lifshitz points of the ANNNXY, ANNNH… models \(^7\) which are intermediate between the ANNNI and the ANNNI model. Since the number of dimensions \( d \) merely enters as a parameter, local scale invariance could also be tested along the lines of an \( \epsilon \)-expansion. \(^16\) Finally, the consistency of other correlators (e.g., energy-energy) with LSI should be tested. We plan to come back to this elsewhere. It would be tempting to see whether the powerful techniques of 2D conformal invariance \(^5\) might be extended to the situation of anisotropic scaling realized at Lifshitz points. This would lead to numerous physical applications \(^8\) and is under investigation.

In conclusion, the precise localisation of the 3D ANNNI model Lifshitz point and improved estimates of its critical exponents allowed 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.

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\(^**\) Laboratoire associé au CNRS UMR 7556

TABLE 1. Critical exponents at the Lifshitz point of the
3D ANNNI model, as obtained from Monte Carlo simulations
(MC), high-temperature series expansion (HT) and renormalized
field theory (FT). The numbers in brackets give the es-
timated error in the last digit(s).

<table>
<thead>
<tr>
<th>(\alpha)</th>
<th>\beta</th>
<th>\gamma</th>
<th>(2-\alpha)/\gamma</th>
<th>\beta/\gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>MC [19]</td>
<td>0.19(2)</td>
<td>1.00(6)</td>
<td>0.14(2)</td>
<td></td>
</tr>
<tr>
<td>HT [20]</td>
<td>0.20(15)</td>
<td>1.01(1)</td>
<td>1.01(1)</td>
<td></td>
</tr>
<tr>
<td>FT [16]</td>
<td>1.27</td>
<td>1.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FT [17]</td>
<td>1.30</td>
<td>1.34(5)</td>
<td>0.175(8)</td>
<td></td>
</tr>
</tbody>
</table>

TABLE 11. Values of the parameters \( p \) and \( \alpha_1 \) computed from
different moment ratios \( \tilde{J}(\{m_i\}; \{n_j\}) \), see text.

<table>
<thead>
<tr>
<th>( m_i )</th>
<th>( n_i )</th>
<th>( p )</th>
<th>( \alpha_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(0, 0.5)</td>
<td>(0.25, 0.25)</td>
<td>-0.102</td>
<td>32.7</td>
</tr>
<tr>
<td>(-0.25, 0.5)</td>
<td>(0.5, 0.5)</td>
<td>-0.125</td>
<td>31.0</td>
</tr>
<tr>
<td>(0.2, -0.9)</td>
<td>(0.0, -0.7)</td>
<td>-0.100</td>
<td>32.8</td>
</tr>
<tr>
<td>(0.2, -0.6, -0.8)</td>
<td>(0.3, -0.4, -0.5)</td>
<td>-0.102</td>
<td>32.8</td>
</tr>
<tr>
<td>(-0.1, -0.6, -0.7)</td>
<td>(-0.4, -0.5, -0.5)</td>
<td>-0.117</td>
<td>33.5</td>
</tr>
</tbody>
</table>

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

FIG. 2. Scaling function \( \Phi(u) \) (see text) versus \( u^{1/2} = (t - t_c^{\text{MC}})^{1/2} \) for \( \kappa = 0.270 \) and \( T = 3.7475 \). Selected Monte Carlo data for a system of \( 200 \times 200 \times 100 \) spins are shown. Constituting the full data set of \( 1.7 \cdot 10^4 \) points for the scaling function \( \Phi(u) \) (gray points) with the analytical prediction eqs. (6.7) following from the assumption of LS1, with \( p = -0.11, \alpha_1 = 33.2 \) and \( b_0 = 0.41 \) (full curve).