Anisotropic scaling and generalized conformal invariance at Lifshitz points

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Abstract

A new variant of the Wolff cluster algorithm is proposed for simulating systems with competing interactions. This method is used in a high-precision study of the Lifshitz point of the 3D ANNNI model. At the Lifshitz point, several critical exponents are found and the anisotropic scaling of the correlators is verified. The functional form of the two-point correlators is shown to be consistent with the predictions of generalized conformal invariance.

Key words: Conformal invariance, Lifshitz point, ANNNI model, correlation function, Wolff algorithm

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Competing interactions are encountered in a large variety of physical systems such as, among others, magnets, alloys or ferroelectrics. These interactions may lead to rich phase diagrams with a multitude of phases as well as to special multicritical points called Lifshitz points (LP). At an LP, a disordered, a uniformly ordered and a periodically ordered phase become indistinguishable [1]. A large number of systems (magnets, ferroelectric liquid crystals, uniaxial ferroelectrics, block copolymers) have been shown to possess an LP.

This kind of systems may be mimicked by spin models with competing interactions. The simplest of these models is the well-known ANNNI (axial next nearest neighbour Ising) model [2,3]. Because of the presence of the competing interactions, previous Monte Carlo studies of the transition(s) from the disordered high-temperature phase to the ordered low-temperature phases exclusively used single-spin flip algorithms [4,5]. Due to the critical slowing-down inherent to these methods, those numerical studies were limited to rather small system sizes. However, large systems are needed for the precise computation of critical quantities, such as critical exponents or critical correlators.

In this contribution, we present a new variant of the Wolff cluster algorithm [6] specifically designed for the simulation of systems with competing interactions near criticality. Similarly, we also generalize the recently proposed method of Evertz and von der Linden for the computation of correlation functions of infinite systems [7] to systems with competing interactions. As an example, we present results obtained at the LP of the three-
dimensional ANNNI model, and we shall concentrate on the LP critical exponents and critical correlators. In particular, our data for the scaling of the two-point correlation functions are consistent with the theoretical predictions of generalized conformal invariance \[8,9\].

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 \[6\]. 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. If \(i\) is a cluster site (with spin \(s_i\) a site \(j\) neighbouring the cluster site \(i\) will be included into the cluster with probability \(p = \frac{1}{2} (1 + \text{sign}(s_i s_j)) (1 - \exp[-2 J/(k_B T)])\)). One ends up with a cluster of spins having all the same sign, see Fig. 1a, and which is flipped as a whole. This kind of same-sign clusters is obviously not adapted to our problem because of the competing interactions.

The modified cluster algorithm we propose for simulating spin models with competing interactions is in the following presented for the ANNNI model. A generalization to other models is straightforward. The Hamiltonian of the 3D ANNNI model is, with \(s_{xyz} = \pm 1\),

\[
H = -J \sum_{xyz} s_{xyz} \left( s_{(x+1)yz} + s_{(y+1)z} + s_{xy(z+1)} \right) + \kappa \sum_{xyz} s_{xyz} s_{xyz(z+2)}
\]

whereas \(J > 0\) and \(\kappa > 0\) are coupling constants. In the axial \(z\)-direction competition between ferromagnetic nearest-neighbour and antiferromagnetic next-nearest-neighbour couplings occurs, leading to a rich phase diagram \[10\].

Our proposed modified cluster algorithm starts with a randomly chosen seed and 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 \(p_a = p\), whereas an axial next-nearest-neighbour site \(k\) with spin \(s_k\) is included with probability \(p_a = \frac{1}{2} (1 - \text{sign}(s_i s_k)) (1 - \exp[-2 \kappa/(k_B T)])\). Thus the final cluster, which will be flipped as a whole, contains spins of both signs, as shown in Fig. 1b. At variance with the traditional Wolff method, the flipped spins are not necessarily connected by nearest-neighbour couplings. Ergodicity and detailed balance are proven as usual. This algorithm works extremely well in the paramagnetic phase, in the ferromagnetic phase and in the vicinity of the LP. It has not yet been subjected to stringent tests in the modulated region where large free energy barriers make simulations very difficult (we point out recent progress achieved in microcanonical simulations of finite ANNNI systems \[11\]). Note that our algorithm differs from the same-sign cluster algorithm proposed by Luijten and Blöte \[12\] for the simulation of systems with long-range interactions.

In an interesting work, Evertz and von der Lin-
The value of the anisotropy exponent $\kappa$ [4]. Having found a reliable value for $\kappa$, the critical temperature $T_\parallel$ is determined precision two-point correlators in spin systems with competing interactions.

In the following, we report results of a large-scale Monte Carlo study of the uniaxial LP encountered in the 3D ANNNI model where the new algorithms introduced above have been used with great success [9]. The whole study took the equivalent of more than two CPU-years on a DEC alpha workstation. For the investigation of LP properties a precise location of this point is mandatory. One possibility to locate this point is given by the structure factor $S(q) = \sum_r \langle S_0 S_r \rangle \exp(i q r)$ as the transition between uniformly ordered and periodically ordered phases shows up as a shift of the maximum of $S(q)$ from $q = 0$ to a non-zero value [4]. Having found a reliable value for $\kappa_L$, the LP critical temperature is then obtained by standard methods. In Table 1, we compare the location of the LP as obtained from our data with previous estimations. Note that Kaski and Selke [5] did not attempt an independent determination of $\kappa_L$ but merely determined $T_L$ for a $\kappa$ in close vicinity to $\kappa_L$ as obtained from a high-temperature (HT) series expansion [13]. From Table 1 the increase in precision is evident.

The uniaxial LP is a strong anisotropic critical point where the correlation lengths parallel and perpendicular to the axial direction diverge with different critical exponents: $\xi_{\parallel,\perp} \sim |T - T_L|^{-\nu_{\parallel,\perp}}$. The value of the anisotropy exponent $\theta = \nu_{\perp}/\nu_{\parallel}$ is in good approximation equal to $1/2$ [14]. In order to take into account the special finite-size effects coming from the anisotropic scaling at the LP [15], large systems of anisotropic shape with $L \times L \times N$ spins with $20 \leq L \leq 240$ and $10 \leq N \leq 100$ have been simulated.

Our estimates for the LP exponents $\alpha, \beta, \gamma$ are given in Table 2. For the first time, these ANNNI model exponents are computed independently. They were found by investigating effective exponents which yield the critical exponents in the limit $T \rightarrow T_L$ [9,16] (provided that finite-size effects can be neglected). Our error bars take into account both the sample averaging and the uncertainty in the location of the LP. The reliability of our data is illustrated by the agreement of the independently estimated exponents $\alpha, \beta$ and $\gamma$ with the scaling relation $\alpha + 2\beta + \gamma = 2$ up to $\approx 0.8\%$. Furthermore, the agreement with a recent two-loop calculation [17] is remarkable.

Fig. 2 summarizes our data obtained for the LP spin-spin correlator $C(r_{\perp}, r_{\parallel}) = \langle S_{r_{\perp}} S_{r_{\parallel}} \rangle$. It shows the scaling function $\Phi(u)$ related to the correlator by

$$ C(r_{\perp}, r_{\parallel}) = r_{\parallel}^{-2x/\gamma} \Phi(r_{\perp}/r_{\parallel}) $$

Table 1

| $\kappa_L$ | $T_L$ |
|-----------|------|
| HT [13]   | $0.270 \pm 0.005$ | $3.73 \pm 0.03$ |
| MC [5]    | $0.265$ | $3.77 \pm 0.02$ |
| present work | $0.270 \pm 0.004$ | $3.7475 \pm 0.005$ |

Table 2

| $\alpha$ | $\beta$ | $\gamma$ | $(2 - \alpha)/\gamma$ | $\beta/\gamma$ |
|----------|--------|--------|----------------|--------|
| MC [5]   | $0.19(2)$ | $1.40(6)$ | $0.14(2)$ | |
| FT [14]  |         |        | $1.27$ | $0.134$ |
| FT [17]  | $0.160$ | $0.220$ | $1.399$ | $1.315$ | $0.157$ |
| present work | $0.18(2)$ | $0.238(5)$ | $1.36(3)$ | $1.34(5)$ | $0.175(8)$ |
and the scaling dimension \( x = (2 + \theta)/(2 + \gamma/\beta) \) \[8,9\]. In this analysis, we use \( \theta = 1/2 \), since the small deviations from this value obtained in recent field-theoretical calculations \[14,17\] are not yet distinguishable from the purely numerical errors in our data. The data shown in Fig. 2 have been obtained after more than five million cluster updates for a system with \( 200 \times 200 \times 100 \) spins. They permit a nice visual test of the data collapse and establish scaling, for the first time also at the LP.

The inset of Fig. 2 is a direct comparison of our numerical data with the theoretical prediction resulting from a generalization of conformal invariance to strong anisotropic criticality \[8\]. Applied to the LP of the 3D ANNNI model, the anisotropic scaling of the two-point correlators could be confirmed directly for the first time. The form of the scaling function is in agreement with the hypothesis of generalized conformal invariance.

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