

# Critical Behaviour of the $3D$ $XY$ -Model: A Monte Carlo Study

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## Abstract

We present the results of a study of the three-dimensional  $XY$ -model on a simple cubic lattice using the single cluster updating algorithm combined with improved estimators. We have measured the susceptibility and the correlation length for various couplings in the high temperature phase on lattices of size up to  $L = 112$ . At the transition temperature we studied the fourth-order cumulant and other cumulant-like quantities on lattices of size up to  $L = 64$ . From our numerical data we obtain for the critical coupling  $K_c = 0.45420(2)$ , and for the static critical exponents  $\gamma/\nu = 1.976(6)$  and  $\nu = 0.662(7)$ .

## I. INTRODUCTION

Three-dimensional classical  $O(N)$  vector models are of great interest, both as simplest statistical models with a continuous symmetry and as a lattice version of the scalar quantum field theory with  $(\vec{\phi}^2)^2$ -interaction. In particular, the 3D  $O(2)$  model, also called the XY-model, is relevant to the critical behaviour of a number of physical systems, such as the phase transition of superfluid  $^4\text{He}$  and magnetic systems with planar spin Hamiltonians. Quantitative knowledge of the critical behaviour of the  $O(N)$  vector models is mostly based on the field theoretic renormalization group techniques at dimension  $D = 3$  [1] and the  $\epsilon$ -expansion [2,3]. Very accurate values of the critical exponents are among the most successful predictions of these approaches. In addition, the analysis of high temperature series expansions [4] provides estimates for the critical temperature of particular lattice models.

Monte Carlo simulations have also succeeded in providing detailed information about the critical behaviour of the 3D  $O(N)$  vector models, but only in the case of the three dimensional Ising model ( $N = 1$ ) [5,6] is an accuracy close to that of analytic calculations reached.

The difficulty encountered in Monte Carlo simulations with local updates is the critical slowing down near a phase transition. Considerable progress has been achieved during the last 6 years with the development of efficient non-local Monte Carlo algorithms which overcome critical slowing down to a large extent [7].

In the present paper we extend previous Monte Carlo studies of the 3D XY model [8,9] where cluster algorithms [10,11] were first applied to simulate this model. These studies were performed on vector computers, using a moderate amount of CPU-time. Since optimal vectorization cannot be reached for cluster algorithms, we used modern RISC stations for the present study. Using about two months of CPU-time we were able to simulate larger lattices and reached a considerably better statistical accuracy than in the previous studies. This accuracy allowed us to control systematic errors in the estimates for the critical coupling and the critical exponents.

This paper is organized as follows. In section 2 we give the definition of the model and describe the cluster updating algorithm, in section 3 we give our results for the high temperature phase, while section 4 contains our data obtained in the critical region. In section 5 we compare our results with those of previous studies.

## II. CLUSTER UPDATE MONTE CARLO OF THE 3D XY-MODEL

We study the XY-model in three dimensions defined by the partition function

$$\mathcal{Z} = \prod_{i \in \Lambda} \int_{S_1} ds_i \exp(K \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j), \quad (1)$$

where  $\vec{s}_i$  is a two dimensional unit vector, the summation is taken over all nearest neighbour pairs of sites  $i$  and  $j$  on a simple cubic lattice  $\Lambda$  and  $K = \frac{J}{k_b T}$  is the coupling, or more precisely, the reduced inverse temperature.

For ferromagnetic interactions  $J > 0$ , the  $XY$ -model has a second-order phase transition separating a low temperature phase with non-zero magnetization from a massive disordered phase at high temperatures. This phase transition can be viewed alternatively as due to Bose condensation of spin waves [12] or the unbinding of vortex strings [13,14].

A major difficulty encountered in Monte Carlo simulation at second-order phase transitions is critical slowing down. The autocorrelation time  $\tau$ , which is roughly the time needed to generate statistical independent configurations, grows as  $\tau \propto L^z$  at criticality, where  $L$  is the linear size of the system and  $z$  is the dynamical critical exponent. Random walk arguments indicate that local updates like the Metropolis algorithm result in  $z = 2$ , which is consistent with the numerical finding for the  $3D$   $XY$ -model [8].

In the case of  $O(N)$  vector models, critical slowing down can be drastically reduced, using cluster algorithms [8,11,9].

In the present work we employ the single cluster algorithm which was introduced by Wolff [11]. Let us shortly recall the steps of the update. First choose randomly a reflection axis in the  $\mathbb{R}^2$  plane. Denote the component of the spin  $\vec{s}_i$  which is parallel to this reflection axis by  $s_i^{\parallel}$  and that which is orthogonal by  $s_i^{\perp}$ . Then choose randomly a site  $i$  of the lattice as a starting point for the cluster  $\mathcal{C}$ . Visit all neighbour sites  $j$  of  $i$ . These sites join the cluster with the probability

$$p(i, j) = 1 - \exp(-K(s_i^{\perp} s_j^{\perp} + |s_i^{\perp} s_j^{\perp}|)). \quad (2)$$

After this is done, visit the neighbours of the new sites in the cluster and add them to the cluster with probability  $p(i, j)$  which is given above. Iterate this step until no new sites enter the cluster. Now flip the sign of all  $s^{\perp}$  contained in the cluster.

### III. NUMERICAL RESULTS IN THE HIGH TEMPERATURE PHASE.

#### A. Observables to be measured

Let us first summarize the definitions of the observables that we studied. The energy density is given by the two-point correlation function  $G(x_i, x_j) = \langle \vec{s}_i \vec{s}_j \rangle$  at distance one

$$E = \frac{1}{3L^3} \sum_{\langle i, j \rangle} \langle \vec{s}_i \vec{s}_j \rangle. \quad (3)$$

The specific heat of the system at constant external field is defined by the derivative of the energy density with respect to the inverse temperature. It can be obtained from the fluctuations of the energy  $H = -\sum_{\langle i, j \rangle} \vec{s}_i \vec{s}_j$

$$C_h = \frac{1}{L^3} \left( \langle H^2 \rangle - \langle H \rangle^2 \right). \quad (4)$$

The magnetic susceptibility  $\chi$  gives the reaction of the magnetization  $m = \sum_{i \in \Lambda} \vec{s}_i$  to an external field. In the high temperature phase one gets

$$\chi = \frac{1}{L^3} \langle m^2 \rangle, \quad (5)$$

since  $\langle m \rangle = 0$ .

Cluster algorithms enable one to reduce the variance of the expectation values in the high temperature phase by using improved estimators [15,16]. The improved estimator of the magnetic susceptibility is given by

$$\chi_{imp} = \left\langle \frac{2}{|\mathcal{C}|} \left( \sum_{i \in \mathcal{C}} s_i^\perp \right)^2 \right\rangle, \quad (6)$$

where  $|\mathcal{C}|$  denotes the number of spins in the cluster  $\mathcal{C}$ .

There are two common definitions of a correlation length  $\xi$ . The exponential correlation length  $\xi_{exp}$  is defined via the decay of the two-point correlation function at large distances

$$\xi_{exp} = \lim_{|x_i - x_j| \rightarrow \infty} \frac{-|x_i - x_j|}{\log G(x_i, x_j)}, \quad (7)$$

which is equal to the inverse mass gap. For the measurement of the exponential correlation length we consider the correlation function

$$\overline{G}(t) \equiv \langle O_0 O_t \rangle \propto \left( \exp\left(\frac{-t}{\xi_{exp}}\right) + \exp\left(\frac{-(L-t)}{\xi_{exp}}\right) \right), \quad (8)$$

of the translational invariant time slice magnetization  $O_t = \sum_i \vec{s}(x_i, t)$ .

The second-moment correlation length is defined by

$$\xi_{2nd} = \left( \frac{(\chi/F) - 1}{4 \sin^2(\pi/L)} \right)^{\frac{1}{2}}, \quad (9)$$

with  $F = \hat{G}(k)|_{|k|=2\pi/L}$ , where  $\hat{G}(k) = \sum_{j \in \Lambda} \langle \exp(ikx_j) \vec{s}_0 \vec{s}_j \rangle$  is the Fourier transform of the two-point correlation function and  $\chi$  the magnetic susceptibility. For more details see for example ref. [17]. The two definitions of the correlation length do not coincide, since in  $\xi_{exp}$  only the first excited state enters, while in the case of  $\xi_{2nd}$  a mixture of the full spectrum is taken into account. However, near the critical point the two quantities should scale in the same way. As for the magnetic susceptibility there exist improved estimators for the two definitions of the correlation length. The improved estimator of the two-point correlation function is given by

$$\langle \vec{s}_i \vec{s}_j \rangle_{imp} = \left\langle \frac{2}{|\mathcal{C}|} \delta_{ij}(\mathcal{C}) s_i^\perp s_j^\perp \right\rangle, \quad (10)$$

where  $\delta_{ij}(\mathcal{C}) = 1$  if  $i$  and  $j$  belong to the same cluster  $\mathcal{C}$ , otherwise  $\delta_{ij}(\mathcal{C}) = 0$  [15,16]. For  $\xi_{2nd}$  one has to provide a  $F_{imp}$ . This is given by the Fourier transform of the improved two-point correlation function [16,18]

$$F_{imp} = \hat{G}(k)_{imp} \Big|_{|k|=\frac{2\pi}{L}}, \quad (11)$$

with

$$\hat{G}(k)_{imp} = \left\langle \frac{2}{|\mathcal{C}|} \left( \left( \sum_{i \in \mathcal{C}} s_i^\perp \cos(kx_i) \right)^2 + \left( \sum_{i \in \mathcal{C}} s_i^\perp \sin(kx_i) \right)^2 \right) \right\rangle. \quad (12)$$

The helicity modulus describes the reaction of the system to a suitable phase twisting field [19]. The lattice definition of the helicity modulus is given by

$$\Upsilon_\mu = \frac{1}{L^3} \left\langle \sum_{\langle i,j \rangle} s_i s_j (\epsilon_{\langle i,j \rangle} \mu)^2 \right\rangle - \frac{K}{L^3} \left\langle \left( \sum_{\langle i,j \rangle} (s_i^1 s_j^2 + s_i^2 s_j^1) \epsilon_{\langle i,j \rangle} \mu \right)^2 \right\rangle, \quad (13)$$

where  $\mu$  is a unit vector in  $x, y$  or  $z$  direction and  $\epsilon_{\langle i,j \rangle}$  the unit vector connecting the sites  $i$  and  $j$  [20].

## B. Monte Carlo Simulations

In order to obtain an estimate of the critical coupling  $K_c$  and determine static critical exponents, we have done 15 simulations at couplings from  $K = 0.4$  up to  $K = 0.452$  on lattices of linear size  $L = 24$  up to  $L = 112$ . The simulation parameter and the results of the runs are given in Tables I and II. The statistics is given in terms of  $N$  measurements taken every  $N_0$  update steps.  $N_0$  is chosen such that approximately  $N_0 \times \langle \mathcal{C} \rangle = L^3$  and hence the whole lattice is updated once for a measurement. We estimated the statistical errors  $\sigma_A$  of expectation values  $\langle A \rangle$  from

$$\sigma_A^2 = \frac{\langle A^2 \rangle - \langle A \rangle^2}{N/(2\tau)} \quad (14)$$

and from a binning analysis. These error estimates were consistent throughout. The statistical error of quantities which contain several expectation values we calculated from Jackknife-blocking [21].

### 1. Finite-size effects

We tried to avoid a finite-size scaling analysis. Hence we had to choose our lattices large enough to ensure that deviations of the values of the observables from the thermodynamic limit values are negligible.

We therefore have measured the energy density  $E$ , the specific heat  $C_h$ , the helicity modulus  $\Upsilon$ , the exponential correlation length  $\xi_{exp}$  and the second-moment correlation length  $\xi_{2nd}$  for fixed coupling  $K = 0.435$  and increasing system size  $L = 4$  up to  $L = 32$ . The results are summarized in Table III. The values of the observables obtained for  $L = 24$  and  $L = 32$  are consistent within error bars. Furthermore, the values of the helicity modulus  $\Upsilon$  for  $L = 24$  and  $L = 32$  are consistent with 0, which is the thermodynamic limit value of the helicity modulus in the high temperature phase. The correlation length at  $K = 0.435$  is approximately 4. Hence we conclude, assuming scaling, that the systematical deviations from the thermodynamic limit are smaller than our statistical errors for  $L/\xi \geq 6$ . This condition is fulfilled by all the simulation parameters of our runs given in Table I.

## 2. Energy density and specific heat

The energy density  $E$  shows, as expected, no singular behaviour close to the critical temperature. In the scaling region the specific heat  $C_h$  should follow

$$C_h = C_{reg} + C_0 \left( \frac{K_c - K}{K_c} \right)^{-\alpha}, \quad (15)$$

where  $C_{reg}$  denotes the regular part of the specific heat and  $\alpha$  is the critical exponent of the specific heat. In order to estimate  $\alpha$  we did a four-parameter least-square fit. However, it was not possible to extract meaningful estimates. The best fit to the data leads to  $K_c = 0.456(2)$ ,  $\alpha = 0.23(13)$  with  $\chi^2/d.o.f. \approx 0.93$  and the relative errors of the constants are about 100%. If we fix the critical coupling to  $K_c = 0.45420$  (this is our estimate obtained at criticality) the quality of the fit gets worse. Therefore we assumed  $\alpha = 0$  and fitted the data following

$$C_h = C_{reg} + C_0 \log \left( \frac{K_c - K}{K_c} \right). \quad (16)$$

The best three-parameter fit to our data leads to  $K_c = 0.4543(4)$ ,  $C_{reg} = -0.49(20)$  and  $C_0 = -1.61(7)$  with  $\chi^2/d.o.f. \approx 0.61$ , where data with  $\xi > 2.5$  are taken into account. This result shows that our data for the specific heat, combined with extended ansätze, are compatible with an  $\alpha = -0.007(6)$  obtained from the hyperscaling relation  $\alpha = 2 - D\nu$  and the estimate  $\nu = 0.669(2)$  from resummed perturbation series [1], but have no predictive power for the exponent  $\alpha$ .

## 3. Magnetic susceptibility

For comparison we give in Table I the results for the standard and the improved susceptibilities. The statistical error of  $\chi_{imp}$  is about 3.5 to 8 times smaller than the error of the standard susceptibility. But one should remark that the statistical error of the standard estimator depends very much on how often one measures. In the following we only discuss the results obtained with the improved estimator. In order to estimate the critical coupling and the susceptibility exponent  $\gamma$  we performed a three-parameter least-square fit following the scaling law

$$\chi = \chi_0 \left( \frac{K_c - K}{K_c} \right)^{-\gamma}. \quad (17)$$

We obtained  $\gamma = 1.324(1)$ ,  $K_c = 0.454170(7)$  and  $\chi_0 = 1.009(2)$  with  $\chi^2/d.o.f. = 0.65$ , when all data are taken into account. In order to test the stability of the results we successively discarded data points with small  $K$ . The results of these fits are summarized in Table IV.  $\chi^2/d.o.f.$  remains small and the results for  $\gamma$ ,  $K_c$  and  $\chi_0$  are consistent within the error bars for all data-sets that we used. But the small  $\chi^2/d.o.f.$  of the fits discussed above, is of course, no proof for the absence of corrections to the scaling. From renormalization group considerations [22] one expects confluent and analytical corrections of the type

$$\chi(K) = \chi_0 \left( \frac{K_c - K}{K_c} \right)^{-\gamma} + \chi_{conf.} \left( \frac{K_c - K}{K_c} \right)^{-\gamma+\Delta_1} + \chi_{anal.} \left( \frac{K_c - K}{K_c} \right)^{-\gamma+1}, \quad (18)$$

with  $\Delta_1 = \omega\nu$ , where  $\nu$  is the critical exponent of the correlation length and  $\omega$  denotes the correction-to-scaling exponent. We fitted our data according to the scaling law with corrections. Since a fit with 6 free parameters is hard to stabilize, we fixed the critical exponents to the values  $\gamma = 1.3160(25)$ ,  $\omega = 0.780(25)$  and  $\nu = 0.669(2)$  which are obtained from resummed perturbation series [1]. Including all the data points in the fit we get  $K_c = 0.454162(9)$ ,  $\chi_0 = 1.058(7)$ ,  $\chi_{conf.} = -0.16 = (6)$  and  $\chi_{anal.} = 0.18(10)$  with  $\chi^2/d.o.f. \approx 0.73$ . The  $\chi_0$  which is obtained from the simple scaling fit (17), and that obtained from the fit allowing corrections to the scaling, differ by a larger amount than their statistical errors. This shows that one cannot interpret a small  $\chi^2/d.o.f.$  as the absence of systematic errors due to an incomplete fit ansatz.

One can also write the scaling relations in terms of the temperature  $T = \frac{1}{K}$ . This leads to

$$\tilde{\chi}(T) = \tilde{\chi}_0 \left( \frac{T - T_c}{T_c} \right)^{-\gamma} \quad (19)$$

and

$$\tilde{\chi}(T) = \tilde{\chi}_0 \left( \frac{T - T_c}{T_c} \right)^{-\gamma} + \tilde{\chi}_{conf.} \left( \frac{T - T_c}{T_c} \right)^{-\gamma+\Delta_1} + \tilde{\chi}_{anal.} \left( \frac{T - T_c}{T_c} \right)^{-\gamma+1} \quad (20)$$

with corrections. We repeated the analysis as done above. Taking all 15 data points into account we get for the simple scaling fit a  $\chi^2/d.o.f. \approx 61.2$ . We again subsequently discarded data points with small  $K$ . A summary of the results is given in Table V. Starting from 5 discarded data points the  $\chi^2/d.o.f.$  becomes approximately 1. But the results obtained for  $K_c$ ,  $\gamma$  and  $\chi_0$  are not consistent with those obtained from the fit according to eq. (17).

Finally, we performed a four-parameter fit to the scaling relation with corrections and fixed values for the exponents. Taking all data points into account we obtain  $K_c = 0.454163(9)$ ,  $\tilde{\chi}_0 = 1.059(7)$ ,  $\tilde{\chi}_{conf.} = -0.17(6)$  and  $\tilde{\chi}_{anal.} = 1.59(10)$  with  $\chi^2/d.o.f. \approx 0.71$ . The results for  $K_c$ ,  $\chi_0$  and  $\chi_{conf.}$  of the fits according to the ansätze (18) and (20) are consistent within the error bars. The ambiguity between the ansatz with  $K$  as variable and that with  $T$  as variable is covered by the analytic corrections.

We conclude that the scaling ansatz (17) fits well if one chooses the coupling  $K$  as the variable. But we also learned that a small  $\chi^2/d.o.f.$  does not exclude systematic errors, due to corrections to the scaling, that are larger than the statistical ones. Hence it is hard to give final estimates obtained from the simple scaling ansatz that also take systematic errors into account. From the ansatz with corrections to the scaling we obtain, assuming  $\gamma = 1.3160(25)$  and  $\Delta_1 = 0.52182$ , the results  $K_c = 0.454162(13)$ ,  $\chi_0 = 1.058(22)$  and  $\chi_{conf.} = -0.16(11)$ , where the uncertainty of  $\gamma$  is taken into account.

We also like to emphasize that the Wegner amplitude  $\chi_{conf.}$  is negative for the fits that take corrections into account. This is in agreement with a field-theoretical renormalization group calculation of Esser and Dohm, which predicts the confluent correction-to-scaling amplitude to be negative for a finite cut-off [23].

#### 4. Correlation length

We extracted  $\xi_{exp}$  from the large distance behaviour of the improved time slice correlation function eq.(8). We therefore considered the effective correlation length, defined by

$$\xi_{eff}(t) = -\ln \frac{\overline{G}(t-1)}{\overline{G}(t)}, \quad (21)$$

where for brevity we have suppressed the contribution due to periodic boundary conditions. As an example, we show in Fig. 1 the results for  $\xi_{eff}(t)$  obtained on a  $112^3$  lattice at  $K = 0.452$ . A single state dominates the correlation function and a plateau sets in around  $t = \xi_{exp}/2$  and extends to  $t = 3\xi_{exp}$ , with no visible degradation due to increasing statistical errors at large  $t$ . As our final estimate for  $\xi_{exp}$  we took self-consistently  $\xi_{eff}(t)$  at the distance  $t = 2\xi_{exp}$ .

In order to calculate  $\xi_{2nd}$  we used the improved version of eq.(9). The advantage of this definition is that no fit is needed to obtain the correlation length. The data of  $\xi_{exp}$  and  $\xi_{2nd}$  are given in Table II. The deviation of  $\xi_{2nd}$  from  $\xi_{exp}$  is about 1% for  $K = 0.40$  and becomes smaller than 0.1% for  $K \geq 0.448$ .

Since the difference of  $\xi_{exp}$  and  $\xi_{2nd}$  is so small, we will discuss only the results of  $\xi_{exp}$  in the following. First we did a three-parameter fit for  $\xi_{exp}$  following the simple scaling ansatz

$$\xi(K) = \xi_0 \left( \frac{K_c - K}{K_c} \right)^{-\nu}. \quad (22)$$

The results are given in Table VI. Taking all data into account, the fit has a large  $\chi^2/d.o.f$  of about 9. Starting with three data points with small  $K$  being discarded, the  $\chi^2/d.o.f$  is close to 1. But still the critical exponent  $\nu$  and the critical coupling systematically tend to smaller values.

If we fit the data to the simple scaling ansatz (22), where the coupling is replaced as variable by the temperature, a similar behaviour is observable. The results are shown in Table VII. Here one also has to discard three data points to obtain a  $\chi^2/d.o.f$  close to 1. But now the estimates of the critical exponent and the critical coupling start at lower values and tend to larger ones.

This indicates that corrections to the simple scaling ansatz have to be taken into account. Therefore we have fitted all data to the scaling relation with corrections given by

$$\xi(K) = \xi_0 \left( \frac{K_c - K}{K_c} \right)^{-\nu} + \xi_{conf.} \left( \frac{K_c - K}{K_c} \right)^{-\nu+\Delta_1} + \xi_{anal.} \left( \frac{K_c - K}{K_c} \right)^{-\nu+1}, \quad (23)$$

whereas, in the case of the magnetic susceptibility,  $\Delta_1 = \omega\nu$ . The four-parameter fit to all data points with the critical exponents fixed to the resummed perturbation series estimates leads to  $K_c = 0.454167(10)$ ,  $\xi_0 = 0.498(2)$ ,  $\xi_{conf.} = -0.10(2)$  and  $\xi_{anal.} = -0.07(4)$  with  $\chi^2/d.o.f. \approx 0.63$ .

We also made a four-parameter fit to the scaling relation with corrections where the coupling is replaced by the temperature. This leads to  $K_c = 0.454165(10)$ ,  $\tilde{\xi}_0 = 0.498(2)$ ,  $\tilde{\xi}_{conf.} = -0.09(2)$ ,  $\tilde{\xi}_{anal.} = 0.24(3)$  with  $\chi^2/d.o.f. \approx 0.63$ .



Taking the uncertainty of  $\nu$  into account, we leave at  $K_c = 0.454166(15)$ ,  $\xi_0 = 0.498(8)$  and  $\xi_{conf.} = -0.10(6)$ .

In summary, we conclude that systematic deviations from the simple scaling ansatz (22) due to corrections to scaling are important for the analysis of the correlation length data in the coupling range that is accessible to Monte Carlo simulations. Thus it is hard to obtain accurate estimates for the critical exponents and the critical coupling from such an approach.

#### IV. NUMERICAL RESULTS AT CRITICALITY

On lattices of the size  $L = 4, 8, 16, 32$  and  $64$  we performed simulations at  $K_0 = 0.45417$  which is the estimate for the critical coupling obtained in the previous section. As in the high temperature simulation the statistics are given in terms of  $N$  measurements taken every  $N_0$  update steps. We have chosen  $N_0$  such that on the average the lattice is updated approximately twice for one measurement. The results of the runs are summarized in Table VIII.

##### A. Phenomenological Renormalization Group

First we determined the critical coupling  $K_c$  and the critical exponent  $\nu$  employing Binder's phenomenological renormalization group method [24]. In addition to the fourth-order cumulant defined on the whole lattice we also studied cumulants defined on subblocks of the lattice. Therefore let us first introduce blockspins

$$S_B = L_B^{1/2(D-2)} \frac{1}{L_B^D} \sum_{i \in B} \vec{s}_i, \quad (24)$$

where  $L_B$  is the size of the block and  $1/2(D-2)$  is the canonical dimension of the field. In particular we studied the fourth-order cumulant

$$U_{L_B} = 1 - \frac{\langle (S_B^2)^2 \rangle}{3 \langle S_B^2 \rangle^2} \quad (25)$$

for  $L_B = L, L/2$  and a nearest neighbour interaction on subblocks

$$NN = \frac{\langle S_{B_1} S_{B_2} \rangle}{\langle S_B^2 \rangle} \quad (26)$$

for  $L_B = L/2$ .

For the extrapolation to couplings  $K$  other than the simulation coupling  $K_0$ , we used the reweighting formula

$$\langle A \rangle(K) = \frac{\sum_i A_i \exp((-K + K_0)H_i)}{\sum_i \exp((-K + K_0)H_i)}, \quad (27)$$

where  $i$  labels the configurations generated according to the Boltzmann-weight at  $K_0$ . We computed the statistical errors from Jackknife binning on the final result of the extrapolated cumulants. The extrapolation only gives good results within a small neighbourhood of the simulation coupling  $K_0$ . This range shrinks with increasing volume of the lattice.

For sufficiently large  $L_B$  the cumulants have a non-trivial fixed point at the critical coupling. When one considers the cumulants as a function of the coupling, the crossings of the curves for different  $L$  provide an estimate for the critical coupling  $K_c$ . As an example we show in Fig. 2 the fourth-order cumulant in a neighbourhood of  $K_c$ . The figure shows that the crossings of the cumulant are well covered by the extrapolation (27). The error bars of  $U_L$  with  $L = 64$  blow up for  $|K - K_0| > 0.001$  while  $|K_{cross} - K_0| = 0.00003$  for  $L = 32$  and  $L = 64$ . The results for the crossings are summarized in Table IX. The given errors are taken from the size of the crossings of the error bars. The convergence of the crossing coupling  $K_{cross}$  towards  $K_c$  should follow

$$K_{cross}(L) = K_c (1 + const.L^{-(\omega + \frac{1}{\nu})}), \quad (28)$$

where  $\omega$  is the correction to scaling exponent [24]. Our data for the crossings of the cumulants did not allow us to perform a two-parameter fit, keeping the exponents fixed, following the above formula. Within the statistical errors the results of the crossings of the fourth-order cumulants on  $L = 8$  and  $L = 16$  up to  $L = 32$  and  $L = 64$  are consistent. The convergence of the crossings of  $NN$  towards  $K_c$  seems to be slower than that of the fourth-order cumulants, but it is interesting to note that the  $K_{cross}$  for the fourth-order cumulant and  $NN$  come from different sides with increasing  $L$ . This is shown in Fig. 3, where the estimates of  $K_{cross}$  versus the lattice size  $L$  are plotted. Our final estimate for the critical coupling is  $K_c = 0.45420(2)$  obtained from the  $L = 32$  and  $L = 64$  crossing of the fourth-order cumulant on the full lattice. Taking into account the fast convergence of the crossings towards  $K_c$ , that is predicted by (28), we conclude that the systematic error of our estimate for  $K_c$  is smaller than the given statistical error.

At the critical coupling  $K_c$  the cumulants converge with increasing lattice size  $L$  to a universal fixed point. The convergence rate is given by [24]

$$U_L(K_c) = U_\infty (1 + const.L^{-\omega}). \quad (29)$$

The results for the cumulants at  $K = 0.45420$ , which is our estimate of critical coupling, are given in Table X. The data did not allow us to perform a two parameter fit with  $\omega$  being fixed. Hence we take the value  $U_L(K_c) = 0.589(2)$  from  $L = 64$  as our final estimate for the fixed point of the fourth-order cumulant on the full lattice, where we now have taken into account the uncertainty of the estimated critical coupling.

We extracted the critical exponent  $\nu$  of the correlation length from the  $L$  dependence of the slope of the fourth-order cumulant at criticality [24]. According to Binder, the scaling relation for the slope of the fourth-order cumulant is given by

$$\left. \frac{\partial U(L, K)}{\partial K} \right|_{K_c} \propto L^{1/\nu}. \quad (30)$$

We evaluated the slopes of the observables  $A$  entering the cumulant  $U$  according to

$$\frac{\partial \langle A \rangle}{\partial K} = \langle AH \rangle - \langle A \rangle \langle H \rangle, \quad (31)$$

where  $A$  is an observable and  $H$  is the energy. The statistical errors are calculated from a Jackknife analysis for the value of the slope. First we estimated the exponent  $\nu$  from different lattices via

$$\nu = \frac{\ln(L_2) - \ln(L_1)}{\ln\left(\left.\frac{\partial A(L_2, K)}{\partial K}\right|_{K_c}\right) - \ln\left(\left.\frac{\partial A(L_1, K)}{\partial K}\right|_{K_c}\right)}. \quad (32)$$

The results are given in Table XI. The estimates for  $\nu$  stemming from  $U_L$  and  $U_{L/2}$  are stable with increasing  $L$  and consistent with each other for  $L \geq 16$ . Therefore we performed a fit according to eq.(30) with  $U_L$  from lattices of the size  $L = 16$  up to  $L = 64$ . We consider the result  $\nu = 0.662(7)$  as our final estimate for the critical exponent of the correlation length.

### B. Magnetic Susceptibility

In order to estimate the ratio  $\gamma/\nu$  of the critical exponents we studied the scaling behaviour of the magnetic susceptibility defined on the full lattice and on subblocks. The dependence of the susceptibility on the lattice size is given by

$$\chi \propto L^{\gamma/\nu} \quad (33)$$

at the critical coupling. We have estimated  $\gamma/\nu$  from pairs of lattices with size  $L_1, L_2$ . The ratio is then given by

$$\frac{\gamma}{\nu} = \frac{\ln(\chi(L_1, K_c)) - \ln(\chi(L_2, K_c))}{\ln(L_1) - \ln(L_2)}. \quad (34)$$

The second column of Table XII shows the estimates of the ratio obtained from the susceptibility defined on the full lattice, while the third column shows the estimates obtained from the blockspin-susceptibility with subblocks of the size  $L/2$ . The estimates for  $\gamma/\nu$  obtained from the subblocks monotonically increase with increasing lattice size  $L$ , while those obtained from the full lattice decrease. The results obtained from the full lattice for  $L \geq 16$  and the result from the subblocks of the largest lattices are consistent within error bars. Hence we take  $\gamma/\nu = 1.976(6)$  as our final result, where statistical as well as systematic errors should be covered. Using the scaling relation  $\eta = 2 - \frac{\gamma}{\nu}$  we obtain for the anomalous dimension  $\eta = 0.024(6)$ .

### C. Hyperscaling and specific heat

In ref. [24] a dangerous irrelevant scaling field  $u$  is proposed as explanation for a possible violation of hyperscaling. Dangerous means that the scaling function of the correlation

length vanishes with some power  $q$  of the vanishing irrelevant scaling field. Hence the correlation length should scale as

$$\xi \propto L^{1+qy_u} \quad (35)$$

at the critical point. Remember that  $y_u$  is negative for an irrelevant scaling field. At  $K_c = 0.45420$ , which we obtained from the analysis of the fourth-order cumulant, we have fitted  $\xi_{2nd}$  to this relation. The reweighted estimates of  $\xi_{2nd}$  are shown in Table XIII. Taking lattices of size  $L = 16$  up to  $L = 64$  into account we estimate  $qy_u = 0.007(2)$  with  $\chi^2/d.o.f. \approx 0.3$  and only statistical errors considered. This indicates that there is no or only very small hyperscaling violation due to a dangerous irrelevant field.

At criticality the specific heat should scale as

$$C_h(L) = C_{reg} + const. L^{\frac{\alpha}{\nu}}, \quad (36)$$

where  $C_{reg}$  denotes the regular part of the specific heat and  $\alpha$  is the critical exponent of the specific heat. Using the critical exponent  $\nu = 0.662(7)$  obtained from the analysis above the hyperscaling relation  $\alpha = 2 - D\nu$  gives  $\alpha = 0.014(21)$ . We also tried to estimate  $\alpha$  via a three-parameter fit, following the finite-size scaling relation. However, we are not able to give a stable estimate for  $\alpha$ .

### D. Helicity modulus

The 3D XY model is assumed to share the same universality class as an interacting Bose fluid, and the helicity modulus  $\Upsilon$  should be proportional to the superfluid density  $\varrho_s$  of the Bose fluid [19]. Near the critical coupling the superfluid density, resp. the helicity modulus should scale as

$$\varrho_s \propto \Upsilon \propto |K - K_c|^v, \quad (37)$$

with  $v$  the critical exponent of the superfluid density. Assuming hyperscaling the Josephson relation reads  $v = (D - 2)\nu$  [19]. Hence the product

$$\Upsilon \cdot L = const \quad (38)$$

should stay constant at the critical point in 3D. To check this prediction we have measured the helicity modulus  $\Upsilon$  on lattices of size  $L = 4$  to  $L = 32$ . The estimator of  $\Upsilon L$  becomes noisy with increasing lattice size. We tried to overcome this problem by measuring more often, which did not remove the problem completely. Hence we skipped the measurement of  $\Upsilon$  for  $L = 64$ . The results, shown in Table XIII, indicate that the above relation holds.

### E. Performance of the Algorithm

The efficiency of a stochastic algorithm is characterized by the autocorrelation time

$$\tau = \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho(t), \quad (39)$$

where the normalized autocorrelation function  $\rho(t)$  of an observable  $A$  is given by

$$\rho(t) = \frac{\langle A_i \cdot A_{i+t} \rangle - \langle A \rangle^2}{\langle A^2 \rangle - \langle A \rangle^2}. \quad (40)$$

We calculated the integrated autocorrelation times  $\tau$  with a self-consistent truncation window of width  $6\tau$  for the energy density  $E$  and the magnetic susceptibility  $\chi$  for lattices with  $L = 4$  up to  $L = 64$  at the coupling  $K = 0.45417$ . In Fig. 4 we show a log-log plot of the integrated autocorrelation times  $\tau$  of the energy density  $E$  and the magnetic susceptibility  $\chi$  versus the lattice size  $L$  given in units of the average number of clusters that is needed to cover the volume of the lattice. Our estimates for the critical dynamical exponents are  $z_E = 0.21(1)$  and  $z_\chi = 0.07(1)$  taking only statistical errors into account. These results are consistent with those of Janke [9].

Finally let us briefly comment on the CPU time: 160 single cluster updates of the  $64^3$  lattice at the coupling  $K = 0.45417$  plus one measurement of the observables took on average 26 sec CPU time on a IBM RISC 6000-550 workstation. All our MC simulations of the 3D XY model together took about two months of CPU-time.

## V. COMPARISON OF OUR RESULTS WITH PREVIOUS STUDIES

In Table XIV we display estimates of critical properties of the 3D XY-model obtained by various methods. Our estimates of  $K_c$  from the scaling fit to the high temperature data and from the phenomenological RG approach are consistent within 2 standard deviations. But only for the result from the phenomenological RG approach are the systematical errors fully under control. Our error of  $K_c$  is about 4 times smaller than that of previous MC studies [8,9], and also about 4 times smaller than that obtained recently [26] from the analysis of a 14th order high temperature series expansion [28]. Recently Butera et al. [27] extended the high temperature series expansion for the sc lattice to the order 17. Their value for the critical coupling is by three times their error estimate smaller than our value.

The error of  $\gamma$  obtained from a fit to the simple scaling ansatz is about 5 times smaller than those of previous MC studies [8,9]; however, the systematical errors are not under control. The value of  $\gamma$  is, within two standard deviations, consistent with the estimate of Ref. [9]. Our estimate of  $\gamma$  is consistent with the value obtained from the high temperature series expansion [25,26,27] and, within two standard deviations, consistent with the value of the  $\epsilon$ -expansion [3] while the very accurate estimate from the resummed perturbation series [1] is smaller than our estimate by three times the quoted error.

Our estimate for  $\nu$  is consistent within error bars with all other estimates we quote in Table XIV. Our quoted error bars are 3.5 times larger than that of ref. [9]. Janke used finite differences to determine the slope of the cumulant [29], while we used fluctuations at a single temperature (31). Furthermore the smallest lattice size  $L = 16$  included in our fit is chosen

to be rather conservative. The most accurate number for  $\nu$  stems from the measurement of the superfluid fraction of  $^4\text{He}$  [30].

In this work we give for the first time an accurate direct MC estimate for the exponent  $\eta$ , the anomalous dimension of the field. The uncertainty of the estimate is comparable with those obtained with field theoretical methods. Our value of the exponent  $\eta$  is consistent with the estimates from the high temperature series expansion [25,26] and with that of the resummed perturbation series [1], but is smaller than the  $\epsilon$ -expansion [3] result by more than twice our error estimate.

Our result for the critical fourth-order cumulant, is consistent with previous MC results [8,9]. But the value obtained from  $\epsilon$ -expansion [31] is off by about 20 times our error estimate that also takes into account systematic errors. Furthermore we provide estimates for the critical fourth order cumulant on subblocks and a nearest neighbour blockspin product  $NV$ . These numbers might be useful in testing other models sharing the  $XY$  universality class.

## VI. CONCLUSIONS

The application of the single cluster algorithm [11], which is almost free of critical slowing down for the  $3D$   $XY$  model, and the extensive use of modern RISC workstations allowed us to increase the statistics as well as the studied lattices sizes considerably compared with previous MC simulations [8,9]. In the high temperature phase of the model we measured correlation length up to 17.58 with an accuracy of about 0.1%. But the analysis of our data for the correlation length and the magnetic susceptibility showed that it is hard to control systematic errors due to confluent and analytic corrections. It seems to be much easier to fight the systematic errors in the phenomenological RG approach. Analytic corrections are absent at the critical point and corrections to the scaling are less harmful, since the relevant length scale at criticality is the lattice size, which can be chosen much larger than the correlation length in the thermodynamic limit of the high temperature phase. From the crossings of the fourth-order cumulant we obtain  $K_c = 0.45420(2)$ , which reduces the error by a factor of about 4 compared with previous MC studies [8,9]. Further improvements of the accuracy of the estimates of the critical coupling and critical exponents seem to be reachable by just increasing the statistics, while keeping the present lattice sizes. The accurate values obtained for critical cumulants could be very useful for testing whether other models share the  $XY$  universality class. Here of course a proper block-spin definition is essential.

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## FIGURES

FIG. 1. The effective correlation length  $\xi_{eff}(t)$  as a function of separation for coupling  $K = 0.452$  on a lattice of size  $L = 112$ .

FIG. 2. Reweighting plot of the Binder cumulant  $U_L$  of the full lattice from the simulation at  $K = 0.45417$ . The dashed lines give the statistical errors obtained by a binning analysis.

FIG. 3. Plot of the convergence of the critical coupling obtained by the cumulant crossing method. Because of the small statistical errors one is able to see systematic convergence of the critical coupling.

FIG. 4. Intergated autocorrelation times  $\tau$  of the energy density  $E$  and the magnetic susceptibility  $\chi$  versus the lattice size  $L$ . The dynamical critical exponent is given by the slopes of the fits.

# TABLES

TABLE I. Results of the energy density  $E$ , the specific heat at constant external field  $C_h$ , the improved susceptibility  $\chi_{imp}$  and the standard susceptibility  $\chi$  obtained from the simulations in the high temperature phase. The parameters of the runs are given in terms of the simulation coupling  $K$ , the linear size of the system  $L$ , and the statistics, with  $N$  the number of measurements taken every  $N_0$  update steps.

$K$	$L$	$N$	$N_0$	$E$	$C_h$	$\chi_{imp}$	$\chi$
0.400	24	20k	0.9k	0.24697(6)	3.17(3)	16.848(14)	16.70(12)
0.410	32	10k	2k	0.25779(5)	3.39(6)	22.108(19)	22.24(32)
0.420	32	10k	1.6k	0.26970(5)	3.65(6)	30.994(29)	31.18(32)
0.425	32	10k	1.2k	0.27605(6)	3.96(7)	38.21(5)	38.47(38)
0.430	32	20k	0.8k	0.28286(4)	4.22(4)	49.12(6)	48.87(36)
0.435	32	20k	0.6k	0.29023(7)	4.57(8)	66.57(15)	66.6(7)
0.437	32	20k	0.4k	0.29329(5)	4.72(6)	77.11(16)	76.9(5)
0.440	32	20k	0.4k	0.29818(5)	5.11(6)	99.50(20)	99.2(7)
0.443	48	21k	1k	0.30336(3)	5.39(7)	136.41(20)	135.8(9)
0.445	48	40k	0.5k	0.30705(3)	5.84(6)	177.04(30)	176.2(9)
0.448	64	25k	1k	0.31303(2)	6.43(8)	299.14(53)	301.0(2.0)
0.449	64	25k	1k	0.315214(18)	6.61(7)	377.75(64)	378.9(2.5)
0.450	96	12k	3k	0.317497(15)	7.02(11)	503.85(85)	506.5(4.6)
0.451	96	12k	2k	0.319854(13)	7.33(10)	722.1(1.3)	724.6(6.5)
0.452	112	12k	2k	0.322446(12)	8.10(14)	1193.0(3.0)	1201.0(10.0)

TABLE II. Results for the correlation lengths  $\xi_{exp}$  and  $\xi_{2nd}$  obtained from the simulations in the high temperature phase.  $\xi_{2nd}/\xi_{exp}$  gives the ratio between the values of the two correlation lengths.

$K$	$L$	$\xi_{2nd}$	$\xi_{exp}$	$\xi_{2nd}/\xi_{exp}$
0.400	24	1.876(1)	1.898(2)	0.9884
0.410	32	2.182(1)	2.202(2)	0.9909
0.420	32	2.624(2)	2.639(2)	0.9943
0.425	32	2.938(2)	2.953(2)	0.9949
0.430	32	3.361(2)	3.375(3)	0.9959
0.435	32	3.947(5)	3.959(5)	0.9969
0.437	32	4.262(5)	4.273(6)	0.9974
0.440	32	4.875(5)	4.885(6)	0.9979
0.443	48	5.746(5)	5.756(6)	0.9983
0.445	48	6.582(6)	6.593(7)	0.9983
0.448	64	8.638(9)	8.645(10)	0.9991
0.449	64	9.738(9)	9.747(10)	0.9991
0.450	96	11.288(10)	11.295(10)	0.9994
0.451	96	13.587(16)	13.594(16)	0.9995
0.452	112	17.570(19)	17.580(20)	0.9994

TABLE III. Results of the energy density  $E$ , the specific heat  $C_h$ , the helicity modulus  $\Upsilon$ , the improved susceptibility  $\chi_{imp}$ , the correlation lengths  $\xi_{exp}$  and  $\xi_{2nd}$  and the ratio  $L/\xi_{2nd}$  obtained from simulations at  $K = 0.435$  with linear system size  $L$ . The statistics is given in terms of  $N$  measurements taken every  $N_0$  update steps.

$L$	$N$	$N_0$	$E$	$C_h$	$\Upsilon$	$\chi_{imp}$	$\xi_{2nd}$	$\xi_{exp}$	$L/\xi_{2nd}$
4	25k	0.1k	0.3621(26)	6.43(13)	0.2180(44)	15.83(21)	2.015(19)	2.08(2)	1.98
8	20k	0.2k	0.3054(26)	6.56(13)	0.0608(16)	43.00(07)	3.228(3)	3.272(4)	2.48
16	20k	0.2k	0.29114(9)	4.92(6)	0.0056(17)	64.31(16)	3.886(6)	3.901(6)	4.12
20	20k	0.3k	0.29049(7)	4.71(5)	0.0031(16)	66.21(14)	3.938(4)	3.949(5)	5.08
24	20k	0.3k	0.29024(7)	4.65(5)	-0.0001(17)	66.55(15)	3.946(6)	3.959(6)	6.08
32	10k	0.6k	0.29013(7)	4.52(9)	0.0009(25)	66.64(15)	3.949(5)	3.960(5)	8.10

TABLE IV. Estimates for the critical coupling  $K_c$ , the static critical exponent  $\gamma$  and the amplitude  $\chi_0$  obtained from a fit of the improved susceptibility  $\chi_{imp}$  to eq.(17).  $\chi^2/d.o.f$  gives the quality of the fit. # denotes the number of discarded data points at small couplings.

#	$K_c$	$\gamma$	$\chi_0$	$\chi^2/d.o.f.$
0	0.454170(7)	1.3241(10)	1.0090(24)	0.65
1	0.454168(8)	1.3238(12)	1.0099(30)	0.69
2	0.454175(9)	1.3252(14)	1.0057(40)	0.49
3	0.454173(10)	1.3248(18)	1.0069(53)	0.53
4	0.454170(11)	1.3239(22)	1.0101(66)	0.52
5	0.454179(14)	1.3264(31)	1.0016(100)	0.41
6	0.454176(15)	1.3256(35)	1.0043(117)	0.44
7	0.454174(17)	1.3251(43)	1.0060(145)	0.52
8	0.454174(19)	1.3250(52)	1.0063(180)	0.65
9	0.454180(24)	1.3272(74)	0.9979(267)	0.81
10	0.454197(42)	1.3337(156)	0.9736(576)	1.11
11	0.454208(58)	1.3384(240)	0.9557(885)	2.14

TABLE V. Estimates for the critical coupling  $K_c$ , the static critical exponent  $\gamma$  and the amplitude  $\chi_0$  obtained from a fit of the improved susceptibility to eq.(19).  $\chi^2/d.o.f$  gives the quality of the fit. # denotes the number of discarded data points at small couplings.

#	$K_c$	$\gamma$	$\hat{\chi}_0$	$\chi^2/d.o.f.$
0	0.453871(6)	1.2351(8)	1.3972(27)	77.1
1	0.453932(7)	1.2471(10)	1.3500(34)	40.0
2	0.453995(8)	1.2604(13)	1.2970(45)	12.8
3	0.454028(9)	1.2683(16)	1.2648(59)	6.98
4	0.454040(10)	1.2733(20)	1.2440(74)	5.27
5	0.454091(13)	1.2849(29)	1.1959(111)	1.39
6	0.454098(14)	1.2871(33)	1.1870(128)	1.31
7	0.454110(16)	1.2907(40)	1.1720(158)	1.08
8	0.454120(18)	1.2938(49)	1.1587(196)	1.02
9	0.454135(23)	1.2991(70)	1.1359(289)	0.99
10	0.454166(42)	1.3112(150)	1.0845(618)	1.06
11	0.454182(59)	1.3177(231)	1.0570(945)	1.98

TABLE VI. Estimates for the critical coupling  $K_c$ , the static critical exponent  $\nu$  and the amplitude  $\xi_0$  obtained from a fit of the exponential correlation length  $\xi_{exp}$  to eq.(22).  $\chi^2/d.o.f$  gives the quality of the fit. # denotes the number of discarded data points at small couplings.

#	$K_c$	$\nu$	$\xi_0$	$\chi^2/d.o.f.$
0	0.454325(9)	0.7029(7)	0.4294(8)	9.2
1	0.454301(9)	0.7003(8)	0.4327(9)	4.9
2	0.454286(10)	0.6985(9)	0.4351(11)	3.6
3	0.454269(11)	0.6964(10)	0.4381(13)	2.0
4	0.454247(12)	0.6933(13)	0.4426(18)	0.66
5	0.454243(14)	0.6927(18)	0.4436(25)	0.71
6	0.454235(16)	0.6914(21)	0.4457(31)	0.59
7	0.454223(18)	0.6895(24)	0.4487(37)	0.31
8	0.454216(20)	0.6882(30)	0.4509(48)	0.25
9	0.454210(24)	0.6870(39)	0.4529(64)	0.26
10	0.454208(46)	0.6866(90)	0.4537(157)	0.39
11	0.454218(66)	0.6890(140)	0.4493(246)	0.74

TABLE VII. Estimates for the critical coupling  $K_c$ , the static critical exponent  $\nu$  and the amplitude  $\tilde{\xi}_0$  obtained from a fit of the exponential correlation length  $\xi_{exp}$  to eq.(22), where the coupling is replaced by the inverse temperature.  $\chi^2/d.o.f$  gives the quality of the fit. # denotes the number of discarded data points at small couplings.

#	$K_c$	$\nu$	$\tilde{\xi}_0$	$\chi^2/d.o.f.$
0	0.454079(8)	0.6612(6)	0.5024(8)	8.5
1	0.454098(8)	0.6632(7)	0.4994(9)	5.3
2	0.454118(9)	0.6656(8)	0.4957(11)	1.7
3	0.454125(10)	0.6665(9)	0.4944(13)	1.5
4	0.454134(11)	0.6677(12)	0.4923(19)	1.4
5	0.454157(14)	0.6711(16)	0.4866(26)	0.18
6	0.454160(15)	0.6717(19)	0.4857(31)	0.16
7	0.454161(17)	0.6717(23)	0.4856(38)	0.19
8	0.454164(20)	0.6723(29)	0.4846(49)	0.22
9	0.454165(24)	0.6724(38)	0.4844(66)	0.29
10	0.454177(45)	0.6750(90)	0.4796(160)	0.38
11	0.454192(65)	0.6783(136)	0.4734(250)	0.65

TABLE VIII. Results of the energy density  $E$ , the specific heat  $C_h$ , the susceptibility  $\chi$  and the second moment correlation length  $\xi_{2nd}$  obtained from simulations at the fixed coupling  $K = 0.45417$  near the final estimate of the critical coupling.  $\tau$  denotes the integrated autocorrelation time of the specified observable, given in units of the average number of clusters needed to cover the volume of the lattice. The statistics is given in terms of  $N$  measurements taken every  $N_0$  update steps.

$L$	$N$	$N_0$	$E$	$\tau_E$	$C_h$	$\chi$	$\tau_\chi$	$\xi_{2nd}$
4	100k	10	0.40440(44)	2.0(1)	6.561(27)	19.095(34)	1.84(5)	2.3104(37)
8	95k	20	0.35585(20)	2.4(1)	8.890(39)	77.80(15)	1.97(5)	4.6852(65)
16	100k	40	0.338945(7)	2.6(1)	10.757(66)	309.95(60)	1.96(7)	9.447(15)
32	83k	80	0.332815(3)	3.1(1)	12.520(73)	1216.0(2.7)	2.11(5)	18.922(38)
64	72k	160	0.330628(2)	3.7(1)	14.35(11)	4732(12)	2.32(7)	37.793(77)

TABLE IX. Estimates for  $K_c(L)$  obtained via Binder's cumulant crossing technique of the reweighted fourth-order cumulants  $U_L$  and  $U_{L/2}$  and nearest neighbour observable  $NN$ .  $L_1 - L_2$  gives the pair of linear lattice sizes which determine the intersection point.

$K_c(L)$			
$L_1 - L_2$	$U_L$	$U_{L/2}$	$NN$
4 - 8	0.4565(4)	0.4617(3)	0.4378(4)
8 - 16	0.4544(2)	0.45457(8)	0.4517(1)
16 - 32	0.45423(5)	0.45424(4)	0.45393(4)
32 - 64	0.45420(2)	0.45421(2)	0.45415(2)

TABLE X. Results for the fourth-order cumulants  $U_L$ ,  $U_{L/2}$  and the nearest neighbour observable  $NN$  at  $K = 0.45420$  obtained with the reweighting technique from the simulations at  $K = 0.45417$ . The errors are obtained by a Jackknife-blocking procedure.

$L$	$U_L$	$U_{L/2}$	$NN$
4	0.59640(42)	0.56860(25)	0.70557(61)
8	0.59134(42)	0.55270(31)	0.77439(45)
16	0.58966(43)	0.55040(32)	0.79925(44)
32	0.58907(50)	0.54974(37)	0.80640(48)
64	0.58909(44)	0.54925(33)	0.80963(49)

TABLE XI. Estimates for the static critical exponent  $\nu$  obtained using eq.(32), where  $A$  is replaced by the fourth-order cumulants  $U_L$  and  $U_{L/2}$  and the nearest neighbour observable  $NN$  with the critical coupling is set to  $K_c = 0.45420$ , the final estimate of the critical coupling.

lattice	$\nu$		
$L_1 - L_2$	$U_L$	$U_{L/2}$	$NN$
4 – 8	0.6496(93)	0.5807(50)	0.8443(86)
8 – 16	0.6799(111)	0.6576(74)	0.7519(76)
16 – 32	0.6649(126)	0.6694(84)	0.6977(68)
32 – 64	0.6584(154)	0.6565(103)	0.6779(83)

TABLE XII. Estimates for the ratio of the static critical exponents  $\gamma/\nu$  obtained using eq.(34). The first column gives the results of the ratio obtained from the susceptibility of the full lattice while the second column is obtained from the susceptibility of the subblocks.  $L_1 - L_2$  gives the pair of lattices, which is used to calculate the ratio of the exponents.

lattice	$\gamma/\nu$	
$L_1 - L_2$	full lattice	subblocks
4 – 8	2.027(4)	1.898(2)
8 – 16	1.996(4)	1.954(3)
16 – 32	1.978(4)	1.966(3)
32 – 64	1.979(5)	1.974(4)

TABLE XIII. Expectation values of the specific heat  $C_h$ , the second moment correlation length  $\xi_{2nd}$ , and the product of the helicity modulus  $\Upsilon$  times the linear size of the system that are reweighted to the final estimate of the critical coupling  $K_c = 0.45420$ . The errors are calculated from a Jackknife analysis.

$L$	$C_h$	$\xi_{2nd}$	$\Upsilon \cdot L$
4	6.561(27)	2.3112(34)	1.090(2)
8	8.877(33)	4.6856(68)	1.091(4)
16	10.704(72)	9.4639(142)	1.12(1)
32	12.564(63)	19.003(34)	1.13(2)
64	14.406(102)	38.25(69)	-

TABLE XIV. Comparison of critical properties determined from various methods. The results given for the simulations of the model in the high temperature phase are obtained from fits according to the simple scaling ansatz with the coupling  $K$  as parameter. For  $\gamma$  and  $\nu$  from Ref. [25] we took the estimates of the fcc lattice, since the errors are smaller than those obtained from the sc lattice.

Method	Ref.	$K_c$	$\gamma$	$\nu$	$\eta$	$U_L$
Phenomenological RG	this work	0.45420(2)	-	0.662(7)	0.024(6)	0.589(2)
High temperature MC	this work	0.454170(7)	1.324(1)	-	-	-
Phenomenological RG	[9]	0.4542(1)	-	0.670(2)	$\approx 0.02$	0.586(1)
High temperature MC	[9]	0.45408(8)	1.316(5)	-	-	-
Phenomenological RG	[8]	-	-	$\approx 0.67$	-	0.590(5)
High temperature MC	[8]	0.45421(8)	1.327(8)	-	-	-
$\epsilon$ -expansion	[3]	-	1.315(7)	0.671(5)	0.040(3)	-
$\epsilon$ -expansion	[31]	-	-	-	-	0.552
Resummed perturbation series	[1]	-	1.3160(25)	0.669(2)	0.033(4)	-
High temperature series	[25]	0.4539(12)	1.323(15)	0.670(7)	0.028(5)	-
High temperature series	[26]	0.45414(7)	1.325	0.673	0.030	-
High temperature series	[27]	0.45406(5)	1.315(9)	0.68(1)	-	-
Experiment $^4\text{He}$	[30]	-	-	0.6705(6)	-	-