# A Monte Carlo study of leading order scaling corrections of $\phi^4$ theory on a three-dimensional lattice

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**Abstract.** We present a Monte Carlo study of the one-component  $\phi^4$  model on a cubic lattice in three dimensions. Leading order scaling corrections are studied using the finite size scaling method. We compute the corrections to scaling exponent  $\omega$  with high precision. We determine the value of the coupling  $\lambda$  at which leading order corrections to scaling vanish. Using this result we obtain estimates for critical exponents that are more precise than those obtained with field-theoretic methods.

#### 1. Introduction

The divergence of quantities like the correlation length  $\xi$  or the magnetic susceptibility  $\chi$  in the neighbourhood of a critical point is described by scaling laws

$$\xi \propto t^{-\nu} \qquad \chi \propto t^{-\gamma} \tag{1}$$

where  $t = |T - T_c|/T_c$  gives the distance from the critical point. However, such scaling laws are valid in this simple form only in an infinitesimal neighbourhood of the critical temperature on infinitely large systems. Monte Carlo simulations, however, are performed with finite systems. Therefore the analysis of the resulting data requires knowledge of corrections to scaling. A similar observation holds for experimental data of critical systems that are taken at a finite distance from the critical temperature.

While renormalization group [1] (see also, e.g., [2]) predicts the structure of corrections qualitatively, an understanding on a quantitative level is needed for the correct interpretation of Monte Carlo or experimental data. From  $\epsilon$ -expansion, perturbation theory in three dimensions and high-temperature series expansions we know that leading corrections are proportional to  $\xi^{-\omega}$ , with  $\omega \approx 0.8$  for the universality class of the three-dimensional Ising model [3–7]. The systematical error that is quoted for  $\omega$  is about 1% to 5%. In a study [8] of universal amplitude ratios of the Ising universality class the uncertainty of the estimate of  $\omega$  turned out to be a major source of systematic errors. Recent Monte Carlo simulations [9, 10] indicate that the value of  $\omega$  could be considerably larger than 0.8. Little is known about subleading corrections to scaling.

In [6, 7] it was suggested that the study of models that interpolate between the Gaussian model and the Ising model should be used to study leading order corrections to scaling. Such models allow one to vary the amplitude of the corrections to scaling. In particular, they allow one to eliminate leading order corrections by a suitable choice of the parameters of the

action (Hamiltonian). This idea was recently implemented in the framework of Monte Carlo simulations and finite size scaling [10, 11].

In this paper we study the one-component  $\phi^4$  (or Landau–Ginzburg) model in three dimensions on a simple cubic lattice. The action is given by

$$S = \sum_{x} \left\{ -2\kappa \sum_{\mu} \phi_{x} \phi_{x+\hat{\mu}} + \phi_{x}^{2} + \lambda (\phi_{x}^{2} - 1)^{2} \right\}$$
(2)

where the field variable  $\phi_x$  is a real number and x labels the lattice sites.  $\mu$  labels the direction and  $\hat{\mu}$  is a unit-vector in  $\mu$ -direction. The Boltzmann factor is  $\exp(-S)$ . For  $\lambda = 0$  we get the Gaussian model on the lattice. In the limit  $\lambda = \infty$  the Ising model is recovered. Following [11], leading order scaling corrections vanish at  $\lambda = 1.0(1)$ . The authors of [10] find  $\lambda \approx 1.145$ .

The aim of the present study is threefold:

- (1) We improve the accuracy of the  $\lambda$  at which leading order scaling corrections vanish. In particular, we give error estimates for the value that is obtained.
- (2) We obtain an accurate estimate of the correction exponent  $\omega$ . By simulating various values of  $\lambda$  we are able to vary the strength of the leading order corrections.
- (3) Finally simulations at the optimal  $\lambda$  yield accurate results for the critical exponents  $\nu$  and  $\eta$ .

In section 2 we discuss how corrections to scaling that arise from the crossover from the Gaussian fixed point to the Wilson–Fisher fixed point can be studied by finite size scaling. The Monte Carlo algorithm is explained in section 3. In section 4 we give an overview of the simulations that have been performed. The analysis of the data is presented in section 5. In section 6 we compare our results with the literature. Finally we give our conclusions and an outlook.

# 2. Scaling corrections and finite size scaling

 $\epsilon$ -expansion [3] tells us that leading corrections to scaling are related to the RG flow from the Gaussian fixed point into the Wilson–Fisher fixed point. In Monte Carlo simulations of lattices with finite size *L* the Binder cumulant

$$U(L,\kappa,\lambda) = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$
(3)

is the most natural quantity to monitor this flow. The magnetization is given by  $m = \sum_{x} \phi_{x}$ .

Since we like to study the flow on the critical surface it is useful to consider a second phenomenological coupling (i.e. a non-trivial quantity that is invariant under RG transformations). We have chosen the ratio of partition functions with periodic and antiperiodic boundary conditions  $Z_a/Z_p$  [12]. Note that partition functions are by construction conserved under RG transformations. Therefore, the ratio of partition functions  $Z_a/Z_p$  is also conserved.

Instead of computing the Binder cumulant at  $\kappa_c$ , it is computed at the  $\kappa$  such that  $Z_a/Z_p$  takes a fixed value on the given lattice. The practical advantage of this method is that no errors are introduced by an inaccurate estimate of  $\kappa_c$  and that due to cross-correlations, the statistical error of the Binder cumulant at fixed  $Z_a/Z_p$  is smaller than that of the Binder cumulant at fixed  $\kappa$ . In the following we will always fix  $Z_a/Z_p = 0.5425$ , which is, according to [10], a good approximation of

$$\lim_{L \to \infty} Z_a / Z_p |_{\kappa_c}.$$
(4)

The Binder cumulant at a fixed value of  $Z_a/Z_p = 0.5425$  means:

$$U(L,\lambda) = U(L,\bar{\kappa}(L,\lambda),\lambda)$$
(5)

where  $\bar{\kappa}(L, \lambda)$  is determined by

$$Z_a/Z_p(L,\bar{\kappa}(L,\lambda),\lambda) = 0.5425.$$
(6)

The fact that there exists a unique RG-trajectory running from the Gaussian fixed point into the Wilson–Fisher fixed point leads to

$$\bar{U}(L,\lambda) = f(a(\lambda)L) + b(\lambda)L^{-x} + \cdots$$
(7)

where we expect  $x \approx 2$ . The function  $a(\lambda)$  goes to 0 as  $\lambda \rightarrow 0$ . For some finite value of  $\lambda$  leading order scaling corrections vanish and *a* diverges. Reparametrizing the scaling function *f* 

$$\tilde{f}(c(\lambda)L^{-\omega}) = f(a(\lambda)L)$$
(8)

and Taylor-expanding yields

$$\bar{U}(L,\lambda) = \bar{U}^* + c_1(\lambda)L^{-\omega} + c_2c_1(\lambda)^2L^{-2\omega} + \cdots.$$
(9)

In addition to the leading correction  $L^{-\omega}$  and powers of it we should expect that corrections of order  $L^{-2}$ ,  $L^{-4}$  and so on, which exist in the lattice version of the Gaussian model, also survive in some form at the Wilson–Fisher fixed point. One example of such a correction is the restoration of the rotational invariance. The result of [13] indicates that such corrections exist almost unaltered at the Wilson–Fisher fixed point.

# 3. The Monte Carlo algorithm

We followed the idea of Brower and Tamayo [14] and used a combination of the cluster algorithm and a local Metropolis algorithm for updating the field. We replaced the Swendsen–Wang cluster algorithm [15] that was used by Brower and Tamayo with the recently proposed wall-cluster algorithm [10]. The cluster algorithm only updates the sign of the field  $\phi$ . Ergodicity of the update scheme is reached by alternating the cluster update with Metropolis updates that allow one to change the modulus of the field  $\phi$ . Below we give the details of the update schemes that were used.

#### 3.1. Metropolis

In order to make the updating scheme ergodic we performed one Metropolis sweep in an update cycle. The proposal for the site x is generated by

$$\phi'_{x} = \phi_{x} + s(r - \frac{1}{2}) \tag{10}$$

where *r* is a random number uniformly distributed in (0, 1] and *s* parametrizes the size of the change. In our study we have chosen s = 3, yielding acceptance rates between 0.4 and 0.6, depending on  $\lambda$ .

# 3.2. Over-relaxation

In order to speed up the updating of the modulus of the field we added  $n_o$  over-relaxation sweeps to the update cycle. A proposal for the field at site x is generated by

$$\phi'_x = 2\kappa \sum_{y \cdot nn \cdot x} \phi_y - \phi_x \tag{11}$$

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where  $y \cdot nn \cdot x$  means that y is a nearest neighbour of x. This proposal keeps

$$S_{Gauss} = \sum_{x} \left[ -2\kappa \sum_{\mu} \phi_x \phi_{x+\hat{\mu}} + \phi_x^2 \right]$$
(12)

constant. This proposal is accepted if the demon variable  $d \in [0, \infty)$  can take over the energy, i.e.  $d' \ge 0$  with

$$d' = d + \lambda (\phi_x^2 - 1)^2 - \lambda (\phi_x'^2 - 1)^2.$$
(13)

This means that we keep the combined action  $S_{com} = S + d$  constant. *d* is set equal to zero at the beginning of the simulation and it is then updated only with the over-relaxation updates.

As a check of the program we measured the expectation value of *d*:

$$\langle d \rangle = \int_0^\infty dx \, \exp(-x)x = 1.$$
 (14)

For example, from our simulation with L = 96 at  $\lambda = 1.1$  we obtained  $\langle d \rangle = 1.000\,003(4)$ .

The acceptance rate of the over-relaxation step depends on  $\lambda$ . For  $\lambda = 0$  the acceptance rate is 1 by construction. For  $\lambda = 1.1$ , where most of our simulations are done, the acceptance rate is still 0.715.

## 3.3. Wall-cluster

We followed the idea of Brower and Tamayo and used the cluster-update only for updating the sign of the field  $\phi$ . For that purpose we consider the system as an Ising model with a link-dependent coupling constant given by  $\beta_{\langle xy \rangle} = 2\kappa |\phi_x| |\phi_y|$ . This results in the link-dependent delete probability

$$p_d(x, y) = \min[1, \exp(-2\beta_{(xy)}\operatorname{sign}(\phi_x)\operatorname{sign}(\phi_y))] = \min[1, \exp(-4\kappa\phi_x\phi_y)].$$
(15)

Given the delete probability there is still freedom in the choice of clusters to be flipped (i.e. the fields of the cluster are multiplied by -1). In the Swendsen–Wang [15] algorithm clusters are flipped with probability  $\frac{1}{2}$ . In Wolff's [16] single-cluster algorithm the cluster that contains a randomly chosen site of the lattice is flipped. Other rules for the selection of the clusters to be flipped can be found in [17]. In this work we used the wall-cluster algorithm introduced in [10]. In this case all clusters which intersect with a randomly chosen two-dimensional plane of the lattice are flipped. In [10] we show that this version of the cluster algorithm is less affected by critical slowing down than the single-cluster algorithm.

#### 4. The simulations

We performed simulations at a large range of  $\lambda$  values and lattice sizes *L*. In table 1 we give an overview of the simulation parameters and the number of measurements for each set of simulation parameters. Most of our simulations were performed on 200 MHz Pentium Pro PCs running under Linux. The program is written in C. As random number generator we used our own implementation of G05CAF of the NAG-library.

Per measurement we performed one Metropolis sweep, one or two over-relaxation sweeps and four or seven wall-cluster updates. The last wall-cluster update in this sequence is also used for the measurement of the boundary variable. The direction of the plane used for the wallcluster is taken from a fixed sequence. First perpendicular to the 1-direction, then perpendicular to the 2-direction, and then perpendicular to the 3-direction and so on. The position of the plane is chosen randomly.

λ	L	$\text{Stat}/3 \times 10^6$
0.1	6, 8, 12, 16, 24, 32, 48	6, 5, 5, 5, 4, 2, 1
0.2	6, 8, 12, 16, 24, 32, 48	6, 5, 5, 5, 4, 2, 1
0.4	6, 8, 10, 12, 14, 16, 18, 20, 24, 32	6, 5, 5, 6, 9, 6, 6, 5, 5, 2
0.7	2, 3, 4, 5, 6, 8, 12, 16, 24	6, 6, 6, 6, 6, 6, 7, 6, 7
0.8	2, 3, 4, 5, 6, 8, 12, 16, 24	6, 6, 6, 6, 6, 6, 5, 5, 5
0.9	2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16	10, 10, 10, 10, 30, 30, 20, 20, 20, 20, 20, 20
1.1	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15,	8, 8, 8, 8, 25, 30, 30, 32, 30, 11, 10, 6, 6, 6,
	16, 18, 20, 22, 24, 28, 32, 40, 48, 64, 96	5, 5, 5, 5.5, 4, 6, 4, 2.5, 2.6, 1, 0.5
1.145	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14,	8, 8, 8, 8, 25, 30, 30, 30, 30, 11, 10, 6, 6,
	15, 16, 18, 20, 24, 32, 48, 64	6, 5, 5, 6, 4, 3, 1.7, 0.5
1.3	2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 16	10, 10, 10, 10, 30, 30, 20, 20, 20, 20, 20, 20
1.4	2, 3, 4, 5, 6, 7, 8, 12, 16, 24	6, 6, 6, 6, 6, 6, 6, 7, 6, 6
1.5	2, 3, 4, 5, 6, 7, 8, 12, 16, 24	6, 6, 6, 6, 6, 6, 5, 5, 5, 5
2.5	6, 8, 12, 16, 24, 32	6, 5, 5, 5, 4, 2

**Table 1.** Summary of simulation parameters. In the first row we give the value of  $\lambda$ , in the second row the lattice size *L* and in the third row the number of measurements divided by  $3 \times 10^6$ .

The update of a single site with Metropolis takes  $2.0 \times 10^{-6}$  s and the over-relaxation  $0.4 \times 10^{-6}$  s. The construction of one site of the cluster takes, on average,  $4.5 \times 10^{-6}$  s.

We computed the integrated autocorrelation times of the observables that were measured. For example, for our largest lattice size L = 96 at  $\lambda = 1.1$  and  $\kappa \approx \kappa_c$ , using one Metropolis sweep, two over-relaxation sweeps and seven wall-cluster updates per measurement, we obtain  $\tau_{\chi} = 3.56(2)$  and  $\tau_b = 1.93(1)$  in units of measurements for the integrated autocorrelation time of the magnetic susceptibility  $\chi$  and the boundary variable, respectively.

The average sum of the sizes of the clusters per volume that are flipped in one update step are fitted with the ansatz  $S/V = CL^x$ . We obtain  $S/V = 1.394(4)L^{-0.4874(7)}$  taking into account L = 48, 64 and L = 96 for  $\lambda = 1.1$  and  $\kappa \approx \kappa_c$ . The  $\chi^2/d.o.f. = 4.9$  is rather large. Taking only L = 64 and L = 96 yields  $S/V = 1.410(8)L^{-0.4901(14)}$ .

This result has to be compared with  $S/V = 1.008(4)L^{-0.527(1)}$  that was found in [10] for the standard Ising model on the cubic lattice. It seems that in the case of the  $\phi^4$  model there are rather strong corrections to the simple power law.

The simulations were performed at  $\kappa_s$  that were the best estimates of  $\bar{\kappa}$  available at the start of the simulations. In order to evaluate observables at  $\kappa$  values different from  $\kappa_s$  we used second-order Taylor expansion in  $\kappa$  at  $\kappa_s$ . We always checked that the error made by truncating the Taylor series was well below the statistical error. The Taylor coefficients were obtained from the simulations.

In total we used about 3.5 years of Pentium Pro CPU-time for these simulations. The runs for  $\lambda = 1.1$ , which turned out to be close to the optimal  $\lambda$ , took about 570 days.

# 5. Analysing the data

## 5.1. The Binder cumulant and corrections to scaling

We analysed the Binder cumulant at  $Z_a/Z_p = 0.5425$  fixed in order to study corrections to scaling and to find the value of  $\lambda$  where leading order corrections to scaling vanish. To get a first impression we have plotted our data for  $\lambda = 0.4, 0.8, 1.1, 1.5$  and 2.5 for  $5 \leq L \leq 24$  in figure 1. For  $\lambda = 0.4$  and  $\lambda = 0.8$ ,  $\overline{U}$  is decreasing with increasing lattice size *L*. For  $\lambda = 1.1$  starting from about L = 10 the value of  $\overline{U}$  stays constant within error bars. Therefore



Figure 1. The Binder cumulant U at  $Z_a/Z_p = 0.5425$  as a function of the lattice size L for  $\lambda = 0.4, 0.8, 1.1, 1.5$  and 2.5.

**Table 2.** Fit results for the Binder cumulant evaluated at  $Z_a/Z_p = 0.5425$  fixed. The ansatz is given in equation (16). We give results for various minimal lattice sizes  $L_{min}$  and maximal distances  $d_{max}$  of  $\bar{U}$  from its fixed point value  $\bar{U}^*$ .  $\omega$  is the correction to scaling exponent.

$L_{min}$	$d_{max}$	$\chi^2/d.o.f.$	$ar{U}^*$	ω
8	0.06	5.36	1.603 51(8)	0.865(3)
8	0.04	2.45	1.603 00(8)	0.866(5)
8	0.03	2.06	1.602 86(8)	0.866(7)
12	0.06	2.02	1.603 98(13)	0.840(5)
12	0.04	1.43	1.603 70(14)	0.856(6)
12	0.03	1.21	1.603 44(15)	0.864(10)
16	0.06	1.85	1.604 35(20)	0.817(8)
16	0.04	1.31	1.603 79(22)	0.853(11)
16	0.03	1.18	1.603 62(23)	0.863(12)

the value of  $\lambda$  at which leading order corrections to scaling vanish should be very close to 1.1. Going to  $\lambda = 1.5$  and  $\lambda = 2.5$ , the value of  $\overline{U}$  is increasing with the lattice size. For a given lattice size,  $\overline{U}$  is monotonically increasing with decreasing  $\lambda$ .

Next we analysed our data for U in a more quantitative fashion. In a first attempt we fitted the data with the simple ansatz

$$\bar{U}(L,\lambda) = \bar{U}^* + c_1(\lambda)L^{-\omega}.$$
(16)

Our fit results are summarized in table 2. The data which are included in the fit are determined by two criteria. First, the lattice size has to be larger than a minimal lattice size  $L \ge L_{min}$ . Second, the distance  $d = |\bar{U}(L, \lambda) - \bar{U}^*|$  has to be smaller than a maximal distance  $d \le d_{max}$ . The first criterion allows one to control effects of higher order corrections in general, while the second specifically controls higher corrections that involve the same scaling field as the leading correction  $(L^{-2\omega}, L^{-3\omega}, ...)$ .

The numbers for  $\chi^2/d.o.f.$  indicate that at least  $L_{min} = 12$  and  $d_{max} = 0.04$  is required to obtain a reliable fit. Results from the fits with a  $\chi^2/d.o.f.$  close to one give  $\omega = 0.85$  up to 0.87 for the correction to scaling exponent. This value is clearly larger than that given by

**Table 3.** Fit results for the Binder cumulant at  $Z_a/Z_p = 0.5425$  fixed. Compared with the previous table a term proportional to  $L^{-2\omega}$  has been included into the ansatz (17).

L <sub>min</sub>	$d_{max}$	$\chi^2/d.o.f.$	$ar{U}^*$	ω	<i>c</i> <sub>2</sub>
8	all	3.08	1.603 18(8)	0.847(2)	-1.01(2)
8	0.07	1.83	1.60276(9)	0.847(3)	-1.64(7)
8	0.05	1.94	1.60277(9)	0.849(4)	-1.57(15)
12	all	1.19	1.603 55(13)	0.839(5)	-1.17(5)
12	0.07	0.95	1.603 28(15)	0.846(6)	-1.57(10)
12	0.05	1.01	1.603 28(16)	0.846(6)	-1.54(29)
16	all	1.02	1.603 63(21)	0.839(9)	-1.31(10)
16	0.07	0.95	1.603 44(23)	0.845(11)	-1.65(18)
16	0.05	1.02	1.603 36(26)	0.845(11)	-1.97(48)

**Table 4.** The correction to scaling amplitude  $c_1(\lambda)$  as a function of  $\lambda$  from fits with the ansatz (17). We give the results for three values of  $L_{min} = 12$ , 14 and 16.  $d_{max} = 0.07$  in all three cases.

λ	$L_{min} = 12$	$L_{min} = 14$	$L_{min} = 16$
0.1	1.452(44)	1.454(61)	1.465(81)
0.2	0.809(21)	0.810(28)	0.812(37)
0.4	0.3882(85)	0.387(12)	0.387(16)
0.7	0.1485(39)	0.1482(52)	0.1462(72)
0.8	0.0985(32)	0.0982(42)	0.0988(59)
0.9	0.0628(22)	0.0623(31)	0.0602(41)
1.1	0.0001(18)	0.0006(25)	-0.0015(34)
1.145	-0.0116(16)	-0.0128(22)	-0.0139(31)
1.3	-0.0479(13)	-0.0481(16)	-0.0482(23)
1.4	-0.0684(18)	-0.0686(19)	-0.0739(30)
1.5	-0.0857(20)	-0.0859(22)	-0.0896(32)
2.5	-0.1933(28)	-0.1934(36)	-0.1944(49)
$\infty$	-0.3112(39)	-0.3113(58)	-0.3125(76)

most recent field theoretic work [5].

Values for  $c_1(\lambda)$  are not listed here. They will be discussed in more detail below. In a second attempt, the data were fitted with the ansatz

$$\bar{U}(L,\lambda) = \bar{U}^* + c_1(\lambda)L^{-\omega} + c_2c_1(\lambda)^2L^{-2\omega}.$$
(17)

The additional term requires only one further parameter in the fit. Our results are summarized in table 3. We note that, as expected, data with much larger values of  $d = \overline{U} - \overline{U}^*$  can be included in the fit. The variation of  $\omega$  with varying  $L_{min}$  and  $d_{max}$  is considerably reduced compared with the previous fit.

As our final result we quote  $\omega = 0.845(10)$ , where we take into account the variation of the result with  $L_{min}$  and  $d_{max}$ .

For a small number of fits we give in table 4 the results for  $c_1(\lambda)$ . We see that for  $\lambda = 1.1$ , within error bars, the leading corrections to scaling vanish. Converting the error bar of  $c_1(\lambda)$  to  $\lambda$  we get  $\lambda_{opt} = 1.100(7)$  from  $L_{min} = 12$ ,  $\lambda_{opt} = 1.102(8)$  from  $L_{min} = 14$ , and  $\lambda_{opt} = 1.095(12)$  from  $L_{min} = 16$ .  $\lambda_{opt}$  is the  $\lambda$  where leading order corrections vanish.

In order to check the existence of the scaling function of equation (7), in figure 2 we have plotted  $\overline{U}$  for  $\lambda = 0.1, 0.2, 0.4, 0.7$ , and 0.8 as a function of

$$L' = \left(\frac{c(\lambda)}{c(0.1)}\right)^{-1/\omega} L.$$
(18)



**Figure 2.** The Binder cumulant U at  $Z_a/Z_p = 0.5425$  as a function of the rescaled lattice size  $L' = a(\lambda)L$  for  $\lambda = 0.1, 0.2, 0.4, 0.7$  and 0.8.

**Table 5.** Fits of the difference of the Binder cumulant at  $\lambda_1 = 0.9$  and  $\lambda_2 = 1.3$  with the ansatz (20). We give  $dc = c_1(\lambda_1) - c_1(\lambda_2)$  and the correction to scaling exponent  $\omega$ .

$L_{min}$	$\chi^2/\text{d.o.f.}$	dc	ω
2	2.84	0.1149(7)	0.870(4)
3	2.83	0.1132(12)	0.862(6)
4	1.18	0.1078(18)	0.838(8)
5	1.26	0.1065(23)	0.833(11)
6	1.39	0.1076(28)	0.837(12)

The values for c are taken from table 4. We see that almost all data points fall nicely on a unique curve. Only for the smallest lattice sizes that have been included (L = 6) is a small deviation visible.

Finally, we studied differences of the Binder cumulant at  $Z_a/Z_p = 0.5425$  fixed for different values of  $\lambda$ . We define

$$\Delta \bar{U}(L,\lambda_1,\lambda_2) = \bar{U}(L,\lambda_1) - \bar{U}(L,\lambda_2).$$
<sup>(19)</sup>

This way  $\bar{U}^*$  is cancelled and we expect

$$\Delta U(L,\lambda_1,\lambda_2) = [c_1(\lambda_1) - c_1(\lambda_2)]L^{-\omega} + \cdots.$$
(20)

As an example, we give in table 5 the results of fits for  $\lambda_1 = 0.9$  and  $\lambda_2 = 1.3$ . The interesting fact is that, starting from  $L_{min} = 4$ , the data are already well fitted by the simple ansatz. Also, the value for  $\omega$  obtained this way is compatible with the result obtained above. This means that subleading corrections depend very little on  $\lambda$  and are, to a large extent, cancelled in  $\Delta \overline{U}$ . Hence, there should be a good chance to study these corrections using perturbation theory.

Here we try to obtain a better understanding of the subleading corrections by looking at the results for small L at  $\lambda = 1.1$  in more detail. Corrections to scaling vanish very rapidly. Starting from L = 9, the result for the Binder cumulant at  $Z_a/Z_p$  fixed is consistent with  $\bar{U}^*$  within the error bars. Fitting

$$\bar{U}(L) - \bar{U}^* = cL^{-x}$$
 (21)

we find  $x \approx 6 \pm 1$  when including lattices of size L = 4 up to L = 8. It is quite surprising that the numerically dominant corrections are governed by such a large exponent and not, as one might expect, by  $x \approx 2$ .

The authors of [18] found that a correction term with a rather large exponent has to be included into the fit ansatz in order to fit the Binder cumulant on small lattices. They suggest that this correction exponent is given by  $2y_h$ , where  $y_h \approx 2.48$  is the RG exponent related with the external field. To check this hypothesis we also looked at the corrections of  $Z_a/Z_p$  at  $\kappa_c$ . It turns out that they vanish as rapidly as the corrections of the Binder cumulant. Hence the observed corrections are related to an irrelevant RG exponent.

# 5.2. The critical line $\kappa_c(\lambda)$

In order to obtain a result for the critical coupling  $\kappa_c$  we fitted our data for the ratio of partition functions  $Z_a/Z_p$  with the ansatz

$$Z_a/Z_p(L,\kappa,\lambda) = Z_a/Z_p^* + \frac{\partial Z_a/Z_p}{\partial \kappa}(\kappa - \kappa_c).$$
<sup>(22)</sup>

For  $\lambda = 1.1$  with  $L_{min} = 12$  we obtain the result  $Z_a/Z_p^* = 0.54243(9)$  and  $2\kappa_c = 0.3750965(4)$ . Increasing the minimal lattice size that is included in the fit to  $L_{min} = 16$  we obtain  $Z_a/Z_p^* = 0.54244(14)$  and  $2\kappa_c = 0.3750966(4)$ . In both cases  $\chi^2$ /d.o.f. is a little larger than  $\frac{1}{2}$ .

The result  $Z_a/Z_p^* = 0.54244(14)$  is consistent with previous estimates  $Z_a/Z_p^* = 0.54334(26)\{27\}$  from the standard Ising model and  $Z_a/Z_p^* = 0.54254(14)[6]\{14\}$  from the spin-1 Ising model [10]. The numbers given in the second and third bracket are estimates of systematic errors caused by subleading corrections. In this work we skipped a detailed analysis of systematic errors. However, it is reasonable to assume that systematic errors are of similar size as for the spin-1 Ising model. The estimate  $2\kappa_c = 0.3750966(4)$  for  $\lambda = 1.1$  will be useful in forthcoming studies of scaling laws.

For the other values of  $\lambda$  we determined  $\kappa_c$  from

$$Z_a/Z_p + \frac{\partial Z_a/Z_p}{\partial \kappa}(\kappa_c - \kappa) = 0.5425.$$
(23)

The results are [0.1, 0.3734095(13)], [0.2, 0.3884251(14)], [0.4, 0.3975837(13)], [0.7, 0.3925302(20)], [0.8, 0.3887757(21)], [0.9, 0.3845113(36)], [1.145, 0.3728926(7)], [1.3, 0.3652233(33)], [1.4, 0.3602789(19)], [1.5, 0.3553854(21)], and [2.5, 0.3134347(16)] for the pairs  $[\lambda, 2\kappa_c]$ .

#### 5.3. The magnetic susceptibility

As definition of the magnetic susceptibility we used

$$\chi = \frac{1}{L^3} \left( \sum_x \phi_x \right)^2.$$
(24)

Following [10,19], we tried to extract the exponent  $\eta$  from the magnetic susceptibility evaluated at  $Z_a/Z_p = 0.5425$  or at U = 1.6034 fixed. In the following, the magnetic susceptibility evaluated at  $Z_a/Z_p$  or at U fixed is denoted by  $\bar{\chi}$ . We fitted our data with the ansatz

$$\bar{\chi}(L) = c + dL^{2-\eta} \tag{25}$$

where *c* is an analytic correction. Note that also corrections that decay like  $L^{-x}$  with  $x \approx 2$  are effectively parametrized by this ansatz.

**Table 6.** Results for  $\eta$  from fitting the magnetic susceptibility at  $Z_a/Z_p = 0.5425$  fixed with the ansatz (25).

$L_{min}$	$\chi^2/d.o.f.$	η	d	с
4	25.05	0.0392(1)	0.9856(3)	-0.724(4)
6	2.73	0.0371(1)	0.9789(4)	-0.577(8)
8	1.23	0.0364(2)	0.9765(7)	-0.504(18)
10	1.23	0.0361(3)	0.9755(9)	-0.46(3)
12	1.33	0.0358(4)	0.9745(14)	-0.40(7)
14	1.29	0.0357(5)	0.9740(18)	-0.35(11)
16	1.00	0.0358(6)	0.9742(21)	-0.35(17)

**Table 7.** Results for  $\eta$  from fitting the magnetic susceptibility at U = 1.6034 fixed with the ansatz (25).

$L_{min}$	$\chi^2/d.o.f.$	η	d	С
4	3.24	0.0345(2)	0.9701(5)	-0.31(1)
6	1.24	0.0356(3)	0.9736(7)	-0.38(1)
8	1.34	0.0359(4)	0.9744(12)	-0.41(3)
10	1.28	0.0365(5)	0.9767(17)	-0.50(6)
12	1.09	0.0370(7)	0.9784(25)	-0.59(12)
14	1.02	0.0368(9)	0.9768(32)	-0.45(20)
16	1.26	0.0366(10)	0.9768(39)	-0.45(31)

**Table 8.** Results for  $\eta$  from fitting the magnetic susceptibility at  $Z_a/Z_p = 0.5425$  fixed with the ansatz (26). Note that the ansatz (26) contains no term for analytic corrections.

$L_{min}$	$\chi^2/d.o.f.$	η	d
12	3.92	0.03357(15)	0.9670(4)
14	2.10	0.03431(18)	0.9688(5)
16	1.35	0.03467(22)	0.9700(7)
20	1.30	0.03497(28)	0.9710(9)
24	1.32	0.03534(37)	0.9724(13)
28	1.60	0.03545(43)	0.9728(15)

First we performed fits for  $\lambda = 1.1$ , where leading corrections to scaling vanish. Results for various  $L_{min}$  are given in table 6 for  $Z_a/Z_p = 0.5425$  fixed and table 7 for U = 1.6034fixed. As before,  $L_{min}$  gives the smallest lattice size that has been taken into account for the fit. The  $\chi^2/d.o.f.$  becomes about 1 for  $L_{min} = 8$  for  $Z_a/Z_p$  fixed, and for  $L_{min} = 6$  for U fixed.

As a check we performed fits without analytic part c for  $Z_a/Z_p = 0.5425$  fixed

$$\bar{\chi}(L) = d L^{2-\eta}.$$
(26)

The results are summarized in table 8. Starting from  $L_{min} = 28$ , the result for  $\eta$  becomes consistent with the results obtained from the fitting equation (25) that includes analytic corrections.

Finally we checked for systematic errors due to residual leading order corrections to scaling at  $\lambda = 1.1$ . For that purpose we fitted the magnetic susceptibility at  $Z_a/Z_p = 0.5425$  for  $\lambda = 0.4, 0.8, 1.5, \text{ and } 2.5 \text{ with } L_{min} = 6 \text{ using the ansatz (25)}$ . The results are  $\eta = 0.0493(4)$ , 0.0407(6), 0.0353(5), and 0.0330(5) for the four values of  $\lambda$ , respectively. From the results for

**Table 9.** Fits of the derivative equation of the Binder cumulant U at  $Z_a/Z_p = 0.5425$  fixed. The ansatz (29) is used. As results we give the exponent of the correlation length  $\nu$  and the constant c.

$L_{min}$	$\chi^2/d.o.f.$	ν	c/2
6	2.10	0.6289(1)	-1.744(1)
8	1.70	0.6292(1)	-1.748(2)
10	1.76	0.6293(2)	-1.750(2)
12	1.48	0.6296(3)	-1.753(3)
14	1.50	0.6299(3)	-1.757(4)
16	1.76	0.6299(4)	-1.756(6)

# $\lambda = 0.8$ and $\lambda = 1.5$ we get the estimate

$$\frac{\Delta\eta_{eff}}{\Delta\lambda} \approx -0.01\tag{27}$$

where  $\eta_{eff}$  denotes the numerical result for  $\eta$  obtained from fitting data for lattice sizes L = 6 up to L = 24.

From the previous section we know that the difference of 1.1 and the values of  $\lambda$  where leading order corrections vanish exactly should be smaller than 0.02. Therefore the systematic error in our final estimate of  $\eta$  due to residual leading order corrections should be smaller than  $0.01 \times 0.02 = 0.0002$ . Note that the lattice sizes used to obtain our final result range from L = 8 up to L = 96.

As a final estimate for  $\eta$  we take the result from fitting the magnetic susceptibility at  $Z_a/Z_p = 0.5425$  with the ansatz (25) and  $L_{min} = 12$ :

$$= 0.0358(4)[5]. \tag{28}$$

The estimate of the systematic error is given in the second bracket. It is obtained from the comparison with the ansatz (26) without analytic corrections and from the discussion above on  $L^{-\omega}$  corrections.

#### 5.4. The exponent v

We compute the exponent  $\nu$  from the slope of the Binder cumulant and the slope of  $Z_a/Z_p$  at  $Z_a/Z_p = 0.5425$  fixed. We fitted our data for  $\lambda = 1.1$  with the simple power law ansatz

$$\frac{\partial U}{\partial \kappa} = c L^{1/\nu}.$$
(29)

In table 9 we give our fit results for various values of the minimal lattice size  $L_{min}$  that is included in the fit. The  $\chi^2$ /d.o.f. becomes reasonably small for  $L_{min} = 12$ . Also, the result for  $\nu$  stays stable when  $L_{min}$  is further increased.

In table 10 we give the analogous results for the slope of  $Z_a/Z_p$ . We see that the  $\chi^2/d.o.f.$  are much larger than for the slope of the Binder cumulant. The value obtained for  $\nu$  is increasing with increasing  $L_{min}$ .

Further, for the spin-1 Ising model the authors of [10] found that the slope of the Binder cumulant is scaling much better than the slope of  $Z_a/Z_p$ .

Therefore, we take the result obtained from fitting the slope of the Binder cumulant with  $L_{min} = 12$ ,  $\nu = 0.6296(3)$  as our final result. In order to check for systematic errors due to residual  $L^{-\omega}$  corrections we fitted our data for the slope of the Binder cumulant at  $\lambda = 0.4, 0.8, 1.5, \text{ and } 2.5$  with  $L_{min} = 8$ . We obtained  $\nu = 0.6363(3), 0.6325(5), 0.6271(4), \text{ and } 0.6241(4)$  for the four values of  $\lambda$ , respectively. From  $\lambda = 0.8$  and 1.5 we obtain

$$\frac{\Delta v_{eff}}{\Delta \lambda} \approx -0.01. \tag{30}$$

**Table 10.** Fits of the derivative of  $Z_a/Z_p$  at  $Z_a/Z_p = 0.5425$  fixed. The ansatz (29) is used. As results we give the exponent of the correlation length  $\nu$  and the constant *c*.

$L_{min}$	$\chi^2/d.o.f.$	ν	<i>c</i> /2
6	117.0	0.6254(1)	-1.1524(4)
8	15.1	0.6273(1)	-1.1673(5)
10	4.9	0.6281(1)	-1.1742(7)
12	2.9	0.6286(1)	-1.1794(12)
14	2.2	0.6290(2)	-1.1830(15)
16	1.9	0.6292(2)	-1.1858(20)

 $v_{eff}$  here means the exponent  $\nu$  obtained from fitting lattices of size L = 8 up to L = 24 with the simple power law equation (29).

From the previous section we know that the difference of 1.1 and the values of  $\lambda$  where leading order corrections vanish exactly should be smaller than 0.02. Therefore, the systematic error in our final estimate of  $\nu$  due to residual leading order corrections should be smaller than  $0.01 \times 0.02 = 0.0002$ . Note that the lattice sizes used to obtain our final result range from L = 12 up to L = 96. We arrive at the final result

$$\nu = 0.6296(3)[4] \tag{31}$$

where the second bracket gives an estimate of systematic errors. It is obtained from the discussion on residual  $L^{-\omega}$  corrections and from the comparison of fits of the slope of the Binder cumulant and of the slope of  $Z_a/Z_p$ .

## 6. Comparison with the literature

There exist exhaustive compilations of results for critical exponents in the literature: see, for example, [5,18]. In table 11 we give only the most recent results, that reflect the state of the art. In [10] the spin-1 model was simulated at parameters where leading order corrections vanish (up to numerical uncertainties). The approach to compute critical exponents is very similar to that of this paper. The results for  $\nu$  and  $\eta$  are consistent with the results of this study. The error bars are of similar size. In [10] the authors found indications that the value of  $\omega$  should be larger than that obtained by field-theoretic methods. However, they were not able to give reliable error estimates. Simulating the  $\phi^4$  model at various values of the coupling constant  $\lambda$  allowed us to vary the strength of the corrections to scaling. Therefore, we were able to give a reliable error-estimate for  $\omega$ .

In [9] the standard Ising model was simulated. The authors also use finite size scaling techniques to compute the exponents. In the analysis of the data, leading order corrections to scaling are taken into account. The final result for  $\nu$  is perfectly consistent with our present result. The error bars are a little larger than ours. The value for  $\eta$  is larger than ours but still compatible when the statistical and systematical errors are taken into account. Their value for the correction exponent  $\omega = 0.87(9)$  is consistent with ours but the error bar is nine times larger than ours.

[9,10] as well as the present work employ finite size scaling methods that were pioneered by Binder [20]. It seems to us that such an approach is more robust than the so-called Monte Carlo renormalization group method [21]. Recent results by Gupta and Tamayo [22], using lattices of a size up to L = 256, are inconsistent with our results. In particular their result for the exponent v is by four times the error-estimate smaller than our result. On the other hand, Blöte *et al* [23] give values that are consistant with ours.

**Table 11.** Recent results for critical exponents obtained with Monte Carlo simulations (MC),  $\epsilon$ -expansion, perturbation theory in three dimensions (3D, PT) and high temperature series expansions. When only  $\nu$  and  $\gamma$  are given in the reference we computed  $\eta$  with the scaling law. These cases are indicated by \*. For a discussion see the text.

Reference	Method	ν	η	ω
This work	MC	0.6296(3)(4)	0.0358(4)(5)	0.845(10)
[10]	MC	0.6298(5)	0.0366(8)	
[9]	MC	0.6294(5)(5)	0.0374(6)(6)	0.87(9)
[22]	MCRG	0.625(1)	0.025(6)	$\approx 0.7$
[23]	MCRG	0.6309(12)	0.038(2)	
[5]	3D, PT	0.6304(13)	0.0335(25)	0.799(11)
[5]	$\epsilon$ , bc	0.6305(25)	0.0365(50)	0.814(18)
[5]	$\epsilon$ , free	0.6290(25)	0.0360(50)	0.814(18)
[25]	HT	0.6308(5)	0.0368(18)*	
[6]	HT	0.632(1)	0.0388(32)*	0.854(80)*
[7]	HT	0.6300(15)	0.0365(56)*	0.825(50)*

The  $\epsilon$ -expansion was invented by Wilson and Fisher [3]. Most recent results obtained from the  $\epsilon$ -expansion and from perturbation theory in three dimensions are given in [5]. The results for  $\nu$  and  $\eta$  obtained from the  $\epsilon$ -expansion are in perfect agreement with our results. However, the error bars are considerably larger than those now obtained from Monte Carlo. The result for  $\omega$  is smaller than ours but still consistent within error bars. Parisi [4] proposed to perform perturbative expansions directly in three dimensions (3D PT). The result given in [5] for  $\nu$  is consistent with ours. The value of  $\eta$  is smaller than ours, but still within the quoted error bars. In both cases our error bars are considerably smaller. The value of the correction exponent  $\omega$  obtained from 3D PT [5] is considerably smaller than our result. The results are inconsistent when the error bars that are quoted are taken into account.

The analysis of high-temperature expansions was the first theoretical method that produced reliable, non-mean-field values for critical exponents of three-dimensional systems. For a review of early work see [24]. Still this method gives results that are competitive in accuracy with Monte Carlo and field-theoretic methods. The authors of [25] claim to have the most accurate results obtained from high-temperature series expansions of the Ising model on the bcc lattice. Their result for  $\nu$  is larger than ours. The quoted error bars do not overlap by a small margin. The authors do not quote a value for  $\eta$  in their paper. For the convenience of the reader we converted  $\gamma = 1.2384(6)$  given for the exponent of the magnetic susceptibility using the scaling relation  $\eta = 2 - \gamma/\nu$ . (Converting our numbers we get  $\gamma = 1.2367(11)$ .) One should note that in this work  $\omega$  as well as  $\beta_c$  is taken as external input for the analysis.

We also give results obtained from the series expansion of two-parameter models that interpolate between the Gaussian and the Ising model, similar to the model considered in this paper. While the results of Nickel and Rehr [7] are in perfect agreement with our numbers (with larger error bars) the value obtained by Chen *et al* [6] for v is clearly larger than ours. Also the value  $\gamma = 1.237(2)$  obtained by Nickel and Rehr is consistent with ours, while  $\gamma = 1.2395(4)$  of Chen *et al* seems too large compared with our result.

The values obtained by Nickel and Rehr as well as by Chen *et al* for the correction to scaling exponent  $\omega$  are consistent with our result. However, the error bars are considerably larger than ours.

Further methods to compute critical exponents ('exact RG', 'coherent anomaly method', etc) are discussed in the literature. These methods tend to give less accurate results and are therefore not discussed here.

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Experimental results have been obtained for binary mixtures of fluids, vapour-fluid systems and uni-axial (anti-)ferromagnetic systems. In general, the results agree with the predictions yielded by the theoretical methods discussed above. However, the results for the exponents are less accurate than the theoretical ones. To give only a few examples: the study of the heat capacity of a aniline-cyclohexane mixture gives  $\alpha = 0.104(11)$  [26]. Using the scaling relation  $d\nu = 2 - \alpha$  we get  $\nu = 0.6320(37)$ . A neutron scattering measurement of an antiferromagnetic FeF<sub>2</sub> system gave  $\nu = 0.64(1)$  and  $\gamma = 1.25(2)$  [27]. For a large collection of experimental results see [18].

## 7. Conclusion and outlook

In this study we determined with high precision the value of the coupling  $\lambda$  for which leading corrections to scaling vanish. This allowed us to obtain results for critical exponents with an accuracy better than that of field-theoretic methods.

The knowledge of the optimal  $\lambda$  can also be used for the study of other universal properties of the model, e.g. universal amplitude ratios, the effective potential.

The programme to eliminate leading order corrections can also be applied to the  $\phi^4$  model with more than one component of the field. The case of two components is of particular interest since it is supposed to be in the same universality class as superfluid helium systems. For this system there exist experimental results for  $\nu$  [28] that are by far more accurate than the existing theoretical predictions.

It would be desirable to extend the programme to subleading corrections. However, these corrections are by far less well understood than leading corrections to scaling. Therefore it is unclear how many and what kind of terms should be included into the action.

However, even if it is not possible to remove higher-order corrections to scaling completely it would be a good check of the reliability of the results to redo the study with a different lattice or with more than a next to nearest neighbour coupling.

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# References

- [1] Wegner F J 1972 Phys. Rev. B 5 4529
- [2] Cardy J 1996 Scaling and Renormalization in Statistical Physics (Cambridge: Cambridge University Press)
- [3] Wilson K G and Fisher M E 1972 Phys. Rev. Lett. 28 240
- [4] Parisi G 1980 J. Stat. Phys. 23 49
- [5] Guida R and Zinn-Justin J 1998 J. Phys. A: Math. Gen. 31 8103 (Guida R and Zinn-Justin J 1998 Preprint cond-mat/9803240)
- [6] Chen J H, Fisher M E and Nickel B G 1982 Phys. Rev. Lett. 48 630 Fisher M E and Chen J H 1985 J. Physique (Paris) 46 1645
- [7] Nickel B G and Rehr J J 1990 J. Stat. Phys. 61 1
- [8] Caselle M and Hasenbusch M 1997 J. Phys. A: Math. Gen. 30 4963
- [9] Ballesteros H G, Fernandez L A, Martin-Mayor V, Parisi G and Ruiz-Lorenzo J J 1999 J. Phys. A: Math. Gen. 32 1
  - (Ballesteros H G, Fernandez L A, Martin-Mayor V, Parisi G and Ruiz-Lorenzo J J 1999 Preprint condmat/9805125)
- [10] Hasenbusch M, Pinn K and Vinti S 1999 Phys. Rev. B 59 11 471
  - (Hasenbusch M, Pinn K and Vinti S 1998 Critical exponents of the 3D Ising universality class from finite size scaling with standard and improved actions *Preprint* hep-lat/9806012)

- Ballesteros H G, Fernandez L A, Martin-Mayor V and Munoz-Sudupe A 1998 *Phys. Lett.* B 441 330 (Ballesteros H G, Fernandez L A, Martin-Mayor V and Munoz-Sudupe A 1998 *Preprint* hep-lat/9805022)
   Hasenbusch M 1002 *Physica* A 107 422
- [12] Hasenbusch M 1993 Physica A 197 423
- [13] Campostrini M, Pelissetto A, Rossi P and Vicari E 1998 Phys. Rev. E 57 184 (Campostrini M, Pelissetto A, Rossi P and Vicari E 1998 Preprint cond-mat/9705086)
- [14] Brower R C and Tamayo P 1989 Phys. Rev. Lett. 62 1087
- [15] Swendsen R H and Wang J-S 1987 Phys. Rev. Lett. 58 86
- [16] Wolff U 1989 Phys. Rev. Lett. 62 361
- [17] Kerler W 1993 Phys. Rev. D 47 1285
- [18] Blöte H W J, Luijten E and Heringa J R 1995 J. Phys. A: Math. Gen. 28 6289
- [19] Ballesteros H G, Fernandez L A, Martin-Mayor V, Munoz-Sudupe A, Parisi G and Ruiz-Lorenzo J J 1997 Phys. Lett. B 400 346
- [20] Binder K 1981 Z. Phys. B 43 119
   Binder K 1981 Phys. Rev. Lett. 47 693
- [21] Ma S K 1976 Phys. Rev. Lett. 37 471
   Pawley G S, Swendsen R H, Wallace D J and Wilson K G 1984 Phys. Rev. B 29 4030
- [22] Gupta R and Tamayo P 1996 Int. J. Mod. Phys. C 7 305 (Gupta R and Tamayo P 1996 Preprint cond-mat/9601048)
- [23] Blöte H W J, Heringa J R, Hoogland A, Meyer E W and Smit T S 1996 Phys. Rev. Lett. 76 2613 (Blöte H W J, Heringa J R, Hoogland A, Meyer E W and Smit T S 1996 Preprint cond-mat/9602020)
- [24] Fisher M E 1967 Rep. Prog. Phys. 30 615
- [25] Butera P and Comi M 1997 Phys. Rev. B 56 8212 (Butera P and Comi M 1997 Preprint hep-lat/9703018)
- [26] Rebillot P F and Jacobs D T 1998 *J. Chem. Phys.* **109** 4009
- [27] Belanger D P and Yoshizawa H 1987 *Phys. Rev.* B **35** 4823
- [28] Lipa J A, Swanson D R, Nissen J, Chui T C P and Israelson U E 1996 Phys. Rev. Lett. 76 944 Goldner L S, Mulders N and Ahlers G 1992 J. Low Temp. Phys. 93 131