High precision Monte Carlo study of the 3D XY-universality class

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Abstract

We present a Monte Carlo study of the two-component $\phi^4$ model on the simple cubic lattice in three dimensions. By suitable tuning of the coupling constant $\lambda$ we eliminate leading order corrections to scaling. High statistics simulations using finite size scaling techniques yield $\nu = 0.6723(3)[8]$ and $\eta = 0.0381(2)[2]$, where the statistical and systematical errors are given in the first and second bracket, respectively. These results are more precise than any previous theoretical estimate of the critical exponents for the 3D XY universality class.

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1 Introduction

The 3D XY universality class is unique in the respect that experimental estimates for critical exponents are more precise than any theoretical estimate. These experiments are performed in the neighbourhood of the super-fluid transition of $^4\text{He}$. The specific heat or the super-fluid density is measured as a function of the temperature [1, 2, 3].

In the present study we try to close the gap between theory and experiment by a high statistics Monte Carlo simulation of the two-component $\phi^4$ (or Landau-Ginzburg) model on a three dimensional simple cubic lattice. The action is given by

$$ S = \sum_x \{-2\kappa \sum_\mu \vec{\phi}_x \vec{\phi}_{x+\hat{\mu}} + \phi_x^2 + \lambda (\phi_x^2 - 1)^2\} , $$

(1)

where the field variable $\vec{\phi}_x$ is a vector with two real components and $x = (x_1, x_2, x_3)$, where $x_i$ is integer, labels the lattice sites. $\mu$ labels the directions 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 XY-model is recovered.

In addition to statistical errors Monte Carlo estimates of critical exponents are affected by systematical errors that result from corrections to scaling. These systematical errors can be reduced (in a finite size scaling study) by increasing the linear size $L$ of the lattices that are simulated. A more elegant approach is to remove corrections by a suitable choice of the action. Recently it was demonstrated that leading order corrections to scaling can be removed by a suitable tuning of the coupling constant $\lambda$ in the one-component $\phi^4$ theory on the lattice [4, 5, 6]. Leading order corrections to scaling are proportional to $\xi^{-\omega} (L^{-\omega}$ in finite size scaling), where $\xi$ is the correlation length and $\omega \approx 0.8$.

The paper is organised as follows: In section 2 we discuss the observables that are measured. In section 3 we explain the algorithm that has been used for the simulation and we summarise the simulation parameters. In section 4 the data are analysed. In section 5 our results for exponents are compared with experimental and theoretical estimates given in the literature. In section 6 we give our conclusions and an outlook.

2 The measured quantities

In the case of the one-component model the Binder cumulant turned out to be a good indicator for corrections to scaling [3]. The Binder cumulant is defined by

$$ U = \frac{\langle (\bar{m}^2)^2 \rangle}{\langle \bar{m}^2 \rangle^2} , $$

(2)

where

$$ \bar{m} = \frac{1}{V} \sum_x \vec{\phi}_x $$

(3)
is the magnetisation per lattice site of a given configuration. The volume is \( V = L^3 \). In the following we will always consider systems with periodic boundary conditions. In ref. [6] the Binder cumulant was computed at a fixed value of the ratio of partition functions \( Z_a/Z_p \). \( Z_a \) is the partition function for anti-periodic boundary conditions and \( Z_p \) for periodic boundary conditions. This ratio can also be computed for an arbitrary number of components. For a simulation of the XY model see ref. [7]. However in the present paper we have replaced \( Z_a/Z_p \) by the dimension-less ratio \( \xi_{2nd}/L \) because the second moment correlation length \( \xi_{2nd} \) is easier to implement as \( Z_a/Z_p \). Note that \( \xi/L \), where \( \xi \) is the exponential correlation length on a strip of width \( L \), was used in the pioneering work of Nightingale [8] on the phenomenological renormalization group approach.

The second moment correlation length is defined by
\[
\xi_{2nd} = \left( \frac{\chi/F - 1}{4 \sin^2(\pi/L)} \right)^{1/2}
\tag{4}
\]
where the magnetic susceptibility is given by
\[
\chi = V \langle \vec{m}^2 \rangle
\tag{5}
\]
and
\[
F = \frac{1}{V} \langle |\sum_x \exp \left( i \frac{2\pi x_1}{L} \vec{\phi}_x \right)|^2 \rangle
\tag{6}
\]
is the Fourier transform of the correlation function at minimal momentum. In the simulation we averaged over all three directions to reduce the statistical error. Note that in the following \( \xi_{2nd} \) is always evaluated at a finite value of \( L \) and not for the thermodynamic limit.

We performed some simulations of the one-component model to compare \( \xi_{2nd}/L \) and \( Z_a/Z_p \). We found that the physical as well as statistical properties of \( \xi_{2nd}/L \) and \( Z_a/Z_p \) are similar.

In order to compute observables in the neighbourhood of the simulation parameter \( \kappa_s \) we computed the first two coefficients of the Taylor expansion in \( \kappa - \kappa_s \). We always checked that the errors made by the truncation of the Taylor series are much smaller than the statistical errors of the quantities that were computed.

3 The Simulations

3.1 The Monte Carlo algorithm

We generalise the idea of Brower and Tamayo [9] to simulate the one-component \( \phi^4 \) theory. They use the Swendsen-Wang cluster algorithm [10] to update the sign of the field \( \phi \). In order to obtain an ergodic update they supplement the cluster-update with a Metropolis update that also allows to update the modulus of the field. In our case we use the single cluster algorithm [11] only to update the direction of the
field. The modulus is updated with the Metropolis algorithm. Let us briefly recall the steps of the single cluster algorithm applied to the two-component $\phi^4$ theory. First a direction $\vec{n}$ is chosen

$$n_1 = \sin(2\pi\theta) \quad , \quad n_2 = \cos(2\pi\theta) \quad ,$$

(7)

where $\theta$ is a random-number that is uniformly distributed in $[0,1)$. Next randomly a site of the lattice is picked as seed of the cluster. The cluster is build recursively. New sites enter the cluster when they freeze onto their neighbours that are already members of the cluster. The freezing probability is $p_f = 1 - p_d$ with

$$p_d = \min \left[1, \exp(-4\kappa (\vec{n}\vec{\phi}_x) (\vec{n}\vec{\phi}_y)) \right] .$$

(8)

The fields of all sites in the cluster are reflected

$$\vec{\phi}'_x = \vec{\phi}_x - 2 (\vec{n}\vec{\phi}_x) \vec{n} .$$

(9)

The modulus of $\vec{\phi}$ is changed with a local Metropolis update. A proposal for the field is generated by

$$\phi'_{i,x} = \phi_{i,x} + s(r_i - 0.5)$$

for $i = 1, 2$, where $r_i$ is a random-number that is uniformly distributed in $[0,1)$. The acceptance probability is given by

$$A = \min[1, \exp(S - S')] ,$$

(11)

where $S$ and $S'$ are the action for the original field and the proposal, respectively. We found that a step-size $s = 2$ yields an acceptance rate of about 50%. In one sweep we go trough the lattice in lexicographic order.

### 3.2 The simulation parameters

We performed simulations at a large range of $\lambda$ values and linear 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 200MHz 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. The total amount of CPU-time used for the simulations was about 3 years on the 200MHz Pentium Pro PCs.

Per measurement we performed one sweep with the Metropolis algorithm and $m$ single cluster updates. The number of cluster updates was chosen roughly proportional to the linear lattice size $L$. For some lattice sizes we searched for the $m$ that gives the optimal performance of the algorithm. For $L = 48$ we found $m = 40$ as optimal.
Table 1: Summary of simulation parameters. In the first row we give the value of \(\lambda\), in the second row the linear lattice size \(L\) and in the third row the number of measurements divided by \(3 \times 10^6\).

| \(\lambda\) | \(L\) | stat/\(3 \times 10^6\) |
|------------|------|-----------------|
| 0.5        | 8,16 | 17.5            |
| 1.0        | 6,8,10,12,14,16,18,20,22,24 | 50,10,10,10,10,10,10,10,10,11 |
| 1.5        | 8,16 | 13.6            |
| 1.7        | 8,12,24 | 15,10,2.5 |
| 1.8        | 3,4,5,6,7,8,9,10,12,16 | 20,67,67,20,40,15,45,30,15,8 |
| 1.9        | 3,4,5,6,7,8,12,16,20,24 | 33,27,20,15,20,10,10,11,10 |
| 1.98       | 8,12,16,20,24 | 20,15,10,11,15 |
| 2.0        | 3,4,5,6,7,8,9,10,11,12,13,14 | 133,67,67,50,25,20,24,20,20,20,20,30 |
| 2.2        | 3,4,5,6,7,8,9,10,12,16,24 | 20,20,25,25,20,16,15,22,10,10 |
| 2.3        | 6,7,8,9,10,11,12,14,16,18,20,22,24 | 50,20,10,10,10,9,10,10,10,10,10,10 |

4 Analysing the data

4.1 The Binder cumulant and corrections to scaling

We analysed the Binder cumulant at \(\xi_{2nd}/L = 0.5927\) fixed. This means that first (at fixed \(\lambda\)) \(\kappa_f\) is computed for that \(\xi_{2nd}/L = 0.5927\). Then the Binder cumulant is computed at \(\kappa_f\). In the following we denote the Binder cumulant at \(\xi_{2nd}/L = 0.5927\) by \(\bar{U}\). From preliminary simulations we know that \(\xi_{2nd}/L = 0.5927\) is a good approximation of \(\xi_{2nd}/L|_{\kappa_c}\) (12).

The advantage of this approach is that we need not to search for \(\kappa_c\) and that due to cross-correlations the statistical error of the Binder cumulant at \(\xi_{2nd}/L = 0.5927\) fixed is smaller than at a given value of \(\kappa\). (See e.g. ref. [12].)

For large \(L\) \(\bar{U}\) approaches a universal constant \(\bar{U}_*\). Leading order corrections are given by

\[\bar{U}(L, \lambda) = \bar{U}_* + c_1(\lambda) \ L^{-\omega}\] (13)

We fitted the data for all values of \(\lambda\) simultaneously with this ansatz. The free parameters of this fit are \(\bar{U}_*\), \(\omega\) and \(c_1(\lambda)\) for each value of \(\lambda\).

The results for various minimal lattice sizes \(L_{\text{min}}\) that have been included in the fit are summarised in table 2. The values for \(\chi^2/\text{d.o.f.}\) stay rather large as \(L_{\text{min}}\) is increased. We could not pin-point a particular problem that caused this effect. On the other hand the result for the exponent \(\omega\) is quite stable as \(L_{\text{min}}\) is varied. As our final result for the correction to scaling exponent we quote \(\omega = 0.79(2)\). It is hard to give reliable estimates for the systematical errors. At least the fact that...
Table 2: Fit results for the Binder cumulant evaluated at $\xi_{2nd}/L = 0.5927$ fixed. The ansatz is given in eq. (13). We give results for various minimal lattice sizes $L_{\text{min}}$, $\omega$ is the correction to scaling exponent.

| $L_{\text{min}}$ | $\chi^2$/d.o.f. | $\bar{U}^*$ | $\omega$ |
|------------------|-----------------|-------------|---------|
| 6                | 5.42            | 1.24357(3)  | 0.786(6) |
| 8                | 2.34            | 1.24324(4)  | 0.775(6) |
| 10               | 2.15            | 1.24311(5)  | 0.788(10)|
| 12               | 1.80            | 1.24297(6)  | 0.782(14)|
| 14               | 1.75            | 1.24279(8)  | 0.790(20)|
| 16               | 1.86            | 1.24274(9)  | 0.819(31)|

the result for $\omega$ stays almost constant starting from $L_{\text{min}} = 6$ indicates that these errors should be small.

For $L_{\text{min}} = 12$, 14 and 16 we give the results for $c_1(\lambda)$ in table 3. Linear interpolation of the result for $c_1$ at $\lambda = 2.0$ and $\lambda = 2.2$ yields $\lambda_{\text{opt}} = 2.046(9)$, 2.086(9) and 2.101(10) for $L_{\text{min}} = 12$, 14 and 16, respectively. Where $\lambda_{\text{opt}}$ is defined by $c(\lambda_{\text{opt}}) = 0$. There is still an increase in $\lambda_{\text{opt}}$ visible as $L_{\text{min}}$ increases. We quote $\lambda_{\text{opt}} = 2.10(1)[5]$ as our final result. As a rough estimate of systematical errors we give (in the square brackets) the difference of the result for $L_{\text{min}} = 12$ and $L_{\text{min}} = 16$.

Table 3: The correction to scaling amplitude $c_1(\lambda)$ as a function of $\lambda$ from fits with the ansatz (13). We give the results for three values of $L_{\text{min}} = 12$, 14 and 16.

| $\lambda$ | $L_{\text{min}} = 12$ | $L_{\text{min}} = 14$ | $L_{\text{min}} = 16$ |
|-----------|---------------------|---------------------|---------------------|
| 0.5       | 0.2152(83)          | 0.2220(122)         | 0.2408(207)         |
| 1.0       | 0.0956(37)          | 0.0999(59)          | 0.1094(101)         |
| 1.5       | 0.0398(21)          | 0.0424(28)          | 0.0464(43)          |
| 1.7       | 0.0229(12)          | 0.0280(32)          | 0.0314(42)          |
| 1.8       | 0.0153(8)           | 0.0186(17)          | 0.0207(23)          |
| 1.9       | 0.0077(8)           | 0.0099(11)          | 0.0114(15)          |
| 1.98      | 0.0038(7)           | 0.0067(11)          | 0.0079(14)          |
| 2.0       | 0.0022(6)           | 0.0043(9)           | 0.0057(13)          |
| 2.2       | -0.0074(7)          | -0.0057(13)         | -0.0056(16)         |
| 4.0       | -0.0604(24)         | -0.0601(37)         | -0.0649(63)         |

Following ref. [4] we tried to fit our data with the extended ansatz

$$\bar{U}(L, \lambda) = \bar{U}^* + c_1(\lambda) L^{-\omega} + c_2 c_1(\lambda)^2 L^{-2\omega}.$$  

(14)
However it turned out that we have too few data with a large difference $\bar{U} - \bar{U}^*$ to resolve $c_2$.

Finally we fitted the difference of the Binder cumulant at $\lambda = 2.0$ and $\lambda = 2.2$ with the ansatz

$$\bar{U}(L, \lambda = 2.0) - \bar{U}(L, \lambda = 2.2) = c \ L^{-\omega}.$$  \hspace{1cm} (15)

Results are given in the table\[\text{4}]. It turns out that the $\chi^2$/d.o.f. becomes order 1 already for the very small $L_{\text{min}} = 3$. Also the value obtained for $\omega$ with this small $L_{\text{min}}$ is consistent with the result obtained above. Hence corrections beyond $L^{-\omega}$ do depend very little on $\lambda$ and are cancelled in $\bar{U}(L, \lambda = 2.0) - \bar{U}(L, \lambda = 2.2)$. The same observation holds in the case of the one-component model \[\text{5}\].

Table 4: Fitting the difference of $\bar{U}$ at $\lambda = 2.0$ and $\lambda = 2.2$ with the ansatz (15).

| $L_{\text{min}}$ | $\omega$ | $c_1(2.0) - c_2(2.2)$ | $\chi^2$/d.o.f. |
|-----------------|----------|---------------------|-----------------|
| 3               | 0.787(18)| 0.0106(3)           | 0.98            |
| 4               | 0.780(31)| 0.0104(5)           | 1.09            |
| 5               | 0.794(43)| 0.0107(9)           | 1.21            |

4.2 The critical line $\kappa_c(\lambda)$

As approximation of the critical $\kappa_c$ we take $\kappa_f$ where $\xi_{2nd}/L = 0.5927$. In table\[\text{5}\] we give the result for the largest lattice size available for each value of $\lambda$ that has been studied. Leading corrections are given by

$$\kappa_f - \kappa_c = a \ L^{-1/\nu} + b \ L^{-1/\nu-\omega} + \ldots.$$  \hspace{1cm} (16)

The constant $a$ should be very small since we have chosen $\xi_{2nd}/L = 0.5927$ as a good approximation of $\xi_{2nd}/L^*$. The value of $b$ depends on $\lambda$ and vanishes at $\lambda_{\text{opt}}$. Nevertheless we assume pessimistically that errors decay with $L^{-1/\nu}$. Systematical errors are then computed by comparing $\kappa_f$ at $L$ with $\kappa_f$ at $L/2$. These errors are given in square brackets. Whenever statistical errors reach a similar size as the systematical ones they are quoted in addition in round brackets.

4.3 The exponent $\eta$

We computed the exponent $\eta$ from the finite size behaviour of the magnetic susceptibility $\chi$ at either $\xi_{2nd}/L = 0.5927$ or $U = 1.243$ fixed. We denote the magnetic susceptibility at $\xi_{2nd}/L$ or $U$ fixed by $\bar{\chi}$. It scales as

$$\bar{\chi} = d \ L^{2-\eta}.$$  \hspace{1cm} (17)
Table 5: Estimates of the critical $\kappa_c$ for all values of $\lambda$ that have been simulated. The value for $\lambda = \infty$ has been taken from ref. [12]. The systematical errors are given in square brackets and statistical errors in round brackets.

| $\lambda$ | $L$  | $2\kappa_c$       |
|-----------|------|-------------------|
| 0         | 16   | 0.33...           |
| 0.5       | 16   | 0.4828[6]         |
| 1.0       | 24   | 0.50754[7]        |
| 1.5       | 16   | 0.51197[7]        |
| 1.7       | 24   | 0.51160[2]        |
| 1.8       | 16   | 0.51115[2]        |
| 1.9       | 24   | 0.510576(2)[7]    |
| 1.98      | 24   | 0.510049(1)[7]    |
| 2.0       | 48   | 0.5099049(6)[9]   |
| 2.2       | 24   | 0.508344(2)[4]    |
| 4.0       | 24   | 0.49243[5]        |
| $\infty$ |      | 0.454165(4)       |

First we analysed our data for $\lambda = 2.0$ which is close to $\lambda_{opt}$ and where we have accumulated most data. Results for $\xi_{2nd}/L$ fixed are given in table 6 and for $U$ fixed in table 7.

In both cases rather large $L_{min}$ are needed to reach a $\chi^2$/d.o.f. close to 1. Since $\bar{\chi}$ at fixed $\xi_{2nd}/L$ has a smaller statistical error than $\bar{\chi}$ at fixed $U$ also the statistical error of $\eta$ is smaller for $\xi_{2nd}/L$ fixed than for $U$ fixed.

Table 6: Fits of the magnetic susceptibility at $\xi_{2nd}/L = 0.5927$ fixed with the ansatz (17).

| $L_{min}$ | $d$       | $\eta$          | $\chi^2$/d.o.f. |
|-----------|-----------|-----------------|-----------------|
| 14        | 1.25629(20) | 0.03667(5)      | 10.28           |
| 24        | 1.25957(50) | 0.03742(11)     | 2.91            |
| 26        | 1.26067(61) | 0.03766(14)     | 0.70            |
| 28        | 1.26117(75) | 0.03777(17)     | 0.40            |

Because we had to go to large $L_{min}$ with the simple ansatz (17) we added an analytic correction

$$\bar{\chi} = c + d L^{2-\eta} \ .$$

(18)

Note that also corrections that decay like $L^{-x}$ with $x \approx 2$ are effectively parametrised by this ansatz. Results for fits with this ansatz are given in table 8 for $\xi_{2nd}/L$ fixed and for $U$ fixed in table 9. We see that a small $\chi^2$/d.o.f. is already reached for $L_{min} = 7$ and $L_{min} = 6$ respectively. Despite the fact that $\chi^2$/d.o.f. of order 1 is
Table 7: Fits of the magnetic susceptibility at $U = 1.243$ fixed with the ansatz (17).

| $L_{\text{min}}$ | $d$      | $\eta$   | $\chi^2 / \text{d.o.f.}$ |
|------------------|----------|----------|--------------------------|
| 14               | 1.2598(6)| 0.03740(16) | 2.27                     |
| 22               | 1.2628(13)| 0.03811(31) | 1.20                     |
| 24               | 1.2644(16)| 0.03845(38) | 0.83                     |
| 26               | 1.2625(20)| 0.03804(46) | 0.29                     |

reached the results for $\eta$ do not match within statistical errors. This is a reminder that a small $\chi^2 / \text{d.o.f.}$ does not imply that systematical errors are of the same size as the statistical ones.

Since the statistical error with $\xi_{2\text{nd}}/L$ fixed is smaller we take our final result from these fits. In order to estimate systematical errors we compare results of fits with the range $L_{\text{min}}, L_{\text{max}}$ and $L'_{\text{min}}, L'_{\text{max}} = 2L_{\text{min}}, 2L_{\text{max}}$. Then the error due to $L^{-2}$ (which we assume to be the leading corrections beyond $L^{-\omega}$) corrections in the second interval should be $1/3$ of the difference of the two results (up to a difference in the distribution of the data with the interval). As our final estimate we take the fit result from $L_{\text{min}} = 14$ and $L_{\text{max}} = 48$. For comparison we fitted with $L_{\text{min}} = 7$ and $L_{\text{max}} = 24$. For this interval we get $\eta = 0.03800(13)$. Hence the systematical error from $L^{-2}$ corrections should be smaller than 0.00012 (taking statistical errors into account).

Table 8: Fits of the magnetic susceptibility at $\xi_{2\text{nd}}/L = 0.5927$ fixed with the extended ansatz (18).

| $L_{\text{min}}$ | $c$      | $d$      | $\eta$   | $\chi^2 / \text{d.o.f.}$ |
|------------------|----------|----------|----------|--------------------------|
| 6                | -0.3602(40) | 1.26187(21)| 0.03784(5) | 2.07                     |
| 7                | -0.3809(68) | 1.26246(26)| 0.03798(6) | 1.33                     |
| 8                | -0.395(11)  | 1.26280(34)| 0.03805(8) | 1.17                     |
| 10               | -0.381(18)  | 1.26254(43)| 0.03800(10)| 1.06                    |
| 12               | -0.393(32)  | 1.26275(62)| 0.03804(14)| 1.21                    |
| 14               | -0.405(43)  | 1.26289(73)| 0.03807(16)| 1.40                    |
| 16               | -0.436(72)  | 1.26330(99)| 0.03815(21)| 1.32                    |

Finally we checked for systematical errors due to residual leading order corrections to scaling at $\lambda = 2.0$. For this purpose we fitted our data for $\lambda = 1.0$ and $\lambda = 4.0$ also with $L_{\text{min}} = 14$ and ansatz (18). We get $\eta = 0.0375(13)$ and $\eta = 0.0373(13)$ respectively. Taking into account the statistical errors we find that

$$\left| \frac{\Delta \eta_{\text{eff}}}{\Delta c_1(\lambda)} \right| < 0.018.$$  \hspace{1cm} (19)
Table 9: Fits of the magnetic susceptibility at $U = 1.243$ fixed with the extended ansatz ($I^8$).

| $L_{min}$ | $c$     | $d$     | $\eta$   | $\chi^2$/d.o.f. |
|-----------|---------|---------|----------|-----------------|
| 4         | -0.464(4) | 1.2651(4) | 0.03845(11) | 3.27            |
| 6         | -0.525(12) | 1.2681(6) | 0.03917(16) | 0.76            |
| 8         | -0.526(30) | 1.2682(10) | 0.03918(23) | 0.85            |
| 10        | -0.553(55) | 1.2688(14) | 0.03931(31) | 0.96            |
| 12        | -0.574(90) | 1.2691(18) | 0.03937(40) | 1.05            |
| 14        | -0.47(13)  | 1.2676(22) | 0.03907(49) | 1.17            |
| 16        | -0.24(23)  | 1.2649(32) | 0.03851(67) | 1.27            |

From the previous section we know that the coefficient $c_1(2.0)$ should be smaller than 0.007. (Taking the fit result for $L_{min} = 16$ plus the statistical error). Therefore the systematical error in our final estimate of $\eta$ due to residual leading order corrections should be smaller than 0.00013. As a check we repeated the error-analysis along the lines of ref. [5] and came up with a similar estimate.

As final estimate for $\eta$ we take the result from fitting the magnetic susceptibility at $\xi_{2nd}/L$ fixed with the ansatz ($I^8$) and $L_{min} = 14$

$$\eta = 0.0381(2)[2] .$$

(20)

The estimate of the systematical error is given in the second bracket. It covers residual $L^{-\omega}$ corrections and higher order corrections.

4.4 The exponent $\nu$

We computed the derivate of the Binder cumulant $U$ with respect to $\kappa$ at the fixed value of the Binder cumulant $U = 1.243$ and at the fixed value of $\xi_{2nd}/L = 0.5927$. These quantities behave as

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

(21)

Results of the fits are summarised in table [10] and [11] for fixed $\xi_{2nd}/L$ and for fixed $U$, respectively. The $\chi^2$/d.o.f. becomes order 1 starting from $L_{min} = 8$ and $L_{min} = 7$ respectively. The statistical errors are slightly smaller in the case of fixed $U$.

As in the case of the exponent $\eta$ we expect in addition to the statistical error systematical errors due to the fact that the coefficient of $L^{-\omega}$ corrections does not vanish exactly and due to sub-leading $L^{-2}$ corrections.

In order to estimate these errors we proceed as in the previous section.

As our final result we take the fit with $L_{min} = 14$ and $L_{max} = 48$ of $\frac{\partial U}{\partial \kappa}$ at fixed $U$. In order to estimate $L^{-2}$ corrections we fitted the data in the interval $L_{min} = 7$ and $L_{max} = 24$. For these lattices sizes we obtain $\nu = 0.6712(2)$. Hence the estimate for a $L^{-2}$ error is $0.0011(5)/3 \approx 0.0005$. 
Table 10: Fits of $\frac{\partial U}{\partial \kappa}$ at $\xi_{2nd}/L$ fixed with the ansatz (21).

| $L_{\text{min}}$ | $c/2$ | $\nu$ | $\chi^2$/d.o.f. |
|------------------|-------|-------|-----------------|
| 6                | -0.5542(5) | 0.6709(1) | 3.82            |
| 7                | -0.5565(6)  | 0.6715(2) | 1.76            |
| 8                | -0.5578(7)  | 0.6719(2) | 1.02            |
| 10               | -0.5586(9)  | 0.6721(2) | 0.96            |
| 12               | -0.5595(11) | 0.6723(3) | 0.80            |
| 14               | -0.5608(13) | 0.6727(4) | 0.65            |
| 16               | -0.5620(18) | 0.6729(5) | 0.69            |
| 20               | -0.5610(24) | 0.6727(6) | 0.63            |
| 24               | -0.5632(36) | 0.6732(9) | 0.50            |

Table 11: Fits of $\frac{\partial U}{\partial \kappa}$ at $U$ fixed with the ansatz (24).

| $L_{\text{min}}$ | $c/2$ | $\nu$ | $\chi^2$/d.o.f. |
|------------------|-------|-------|-----------------|
| 6                | -0.5551(4) | 0.6712(1) | 2.07            |
| 7                | -0.5564(5)  | 0.6716(1) | 1.19            |
| 8                | -0.5572(6)  | 0.6718(2) | 0.80            |
| 10               | -0.5577(7)  | 0.6719(2) | 0.73            |
| 12               | -0.5583(9)  | 0.6721(3) | 0.62            |
| 14               | -0.5593(11) | 0.6723(3) | 0.51            |
| 16               | -0.5601(15) | 0.6725(4) | 0.55            |
| 20               | -0.5592(21) | 0.6723(5) | 0.48            |
| 24               | -0.5610(31) | 0.6727(7) | 0.30            |

In order to estimate the error due to residual $L^{-\omega}$ corrections we fitted our data for $\lambda = 1.0$ and $\lambda = 4.0$. From $L_{\text{min}} = 14$ we obtain $\nu = 0.6706(11)$ for $\lambda = 1.0$ and $\nu = 0.6758(10)$ for $\lambda = 4.0$. Hence

$$\left| \frac{\Delta \nu_{\text{eff}}}{\Delta c_1(\lambda)} \right| < 0.04 .$$

From the previous section we know that $c_1(2.0) \approx 0.007$. Therefore the estimate of the systematical error in $\nu$ is $0.04 \times 0.007 \approx 0.0003$.

We arrive at our final estimate

$$\nu = 0.6723(3)[8] ,$$

where the statistical error is given in the first bracket and the systematical error that is given in the second bracket covers $L^{-2}$ and residual $L^{-\omega}$ corrections.
5 Comparison with the literature

In table [12] we give for comparison recent results for critical exponents. Critical exponents for the XY-universality class have been calculated using the high temperature series expansions, the $\epsilon$-expansion, perturbation theory in three dimension and Monte Carlo simulations. Our result for $\nu$ is consistent within error-bars with (almost) all other theoretical results given in table [12]. The result of the MC study [14] seems to be a little too small. Our error-bar is smaller than that of all previous estimates. Our estimate for $\eta$ is consistent with the other theoretical estimates except with the Monte Carlo results. The values of refs. [13, 14] are too small compared with our present estimate. Note that in these studies no careful check of systematical errors due to corrections to scaling was performed. On the other hand the result of ref. [12], which takes into account $L^{-\omega}$ corrections, is by two standard deviations larger than our result.

In contrast to the one-component case [6] our result for the correction to scaling exponent $\omega$ is consistent with that obtained with field theoretic methods.

Table 12: 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 *. In ref. [4] a result for $\alpha$ is given. In the table it is converted to $\nu$ using the scaling relation $\alpha = 2 - d\nu$. For a discussion see the text.

| Ref. | Method | $\nu$ | $\eta$ | $\omega$ |
|------|--------|-------|--------|----------|
| present work | MC | 0.6723(3)[8] | 0.0381(2)[2] | 0.79(2) |
| 13 | MC | 0.670(2) | | |
| 14 | MC | 0.662(7) | 0.026(6) | |
| 12 | MC | 0.6721(13) | 0.042(2) | |
| 15 | 3D,PT | 0.6703(15) | 0.0354(25) | 0.789(11) |
| 15 | $\epsilon$,bc | 0.6680(35) | 0.0380(50) | 0.802(18) |
| 15 | $\epsilon$,free | 0.671 | 0.0370 | 0.802(18) |
| 16 | HT | 0.674(2) | 0.039(7)* | |
| 1 | $^4$He | 0.67095(13) | |
| 1 | $^4$He | 0.6705(6) | |
| 3 | $^4$He | 0.6708(4) | |

Experimental results for the exponent $\nu$ have been obtained for the $\lambda$-transition of $^4$He. These results have smaller error-bars than our Monte Carlo result. The experimental results are all smaller then our value but still the error-bars touch.
6 Conclusion and outlook

In this paper we have improved the accuracy of the theoretical estimate of $\nu$ of the 3D XY universality class considerably. In particular we give in addition to the statistical error a careful estimate of systematical errors that are caused by corrections to scaling. Our value $\nu = 0.6723(3)$ is consistent with other theoretical estimates. However it is larger than the experimental results obtained from the $\lambda$-transition of $^4$He \cite{1,2,3} that give values from 0.6704 up to 0.6709 with an error in the last digit. It would be interesting to further improve the theoretical estimate to the claimed accuracy of the experimental results. This could be achieved by simulating at our best estimate for $\lambda_{opt} = 2.1$ and going to linear lattice sizes roughly twice as large as in the present study to reduce the effect of sub-leading corrections. At a sustained statistical accuracy this would require about 10 years of CPU-time on a modern PC.

In addition to critical exponents amplitude ratios are universal and have been experimentally determined for the $\lambda$-transition of $^4$He. For example the specific heat behaves in the neighbourhood of the phase transition as

$$C = A_{\pm} |t|^{-\alpha} (1 + D_{\pm} |t|^\theta + E_{\pm} t) + B \ ,$$

where $t = (T - T_c)/T_c$ is the reduced temperature. The constants $A_{\pm}, D_{\pm}, E_{\pm}$ and $B$ depend on the system that is considered. The subscript $\pm$ indicates the low and high temperature phase. However renormalization group predicts the ratio $A_+/A_-$ to be universal. Setting $\lambda = \lambda_{opt}$ leads to $D_{\pm} = 0$ which greatly simplifies the determination of $A_+/A_-$ in a Monte Carlo simulation.

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