The three-dimensional $XY$ universality class: a high precision Monte Carlo estimate of the universal amplitude ratio $A_+/A_-$

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Abstract. We simulate the improved three-dimensional two-component $\phi^4$ model on the simple cubic lattice in the low and the high temperature phase for reduced temperatures down to $|T - T_c|/T_c \approx 0.0017$ on lattices of size up to $350^3$. Our new results for the internal energy and the specific heat are combined with the accurate estimates of $\beta_c$ and data for the internal energy and the specific heat at $\beta_c$ recently obtained in Campostrini et al (2006 Preprint cond-mat/0605083). We find $R_\alpha = (1 - A_+/A_-)/\alpha = 4.01(5)$, where $\alpha$ is the critical exponent of the specific heat and $A_\pm$ is the amplitude of the specific heat in the high and the low temperature phase, respectively.

Keywords: classical Monte Carlo simulations, classical phase transitions (theory), critical exponents and amplitudes (theory), finite-size scaling

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The three-dimensional \(XY\) universality class

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1. Introduction

The renormalization group (RG) theory of critical phenomena classifies continuous phase transitions into so called universality classes, which are characterized by the dimension of the system, the range of the interaction, the symmetry of the order parameter and the symmetry-breaking pattern; see e.g. \[2\]–\[5\]. At continuous phase transitions, thermodynamic quantities follow power laws. For example, the specific heat behaves as

\[
C \simeq A_{\pm} |t|^{-\alpha}(1 + c_{\pm} |t|^\theta + \cdots) + c_{\mathrm{ns}},
\]

where \(\alpha\) is the critical exponent of the specific heat, \(\theta\) the exponent of the leading correction to scaling, \(A_+, A_-, c_+, c_-\) are amplitudes in the high and low temperature phases, respectively. The reduced temperature \(t = (T - T_c)/T_c\) gives the distance from the critical temperature \(T_c\). \(c_{\mathrm{ns}}\) is the analytic background, which has to be taken into account when \(\alpha \leq 0\), as is the case here. Following the RG theory, critical exponents are universal, which means that they take exactly the same value for any system within a given universality class. Most recent estimates are \(\alpha = -0.0151(3)\) and \(\theta = 0.527(13)\) \[1\]. For reviews on theoretical and experimental results see \[6,7\]. In addition to the critical exponents, amplitude ratios like \(A_+/A_-\) and \(c_+/c_-\) are universal, while the individual values of \(A_+, A_-, c_+\) and \(c_-\) depend on the microscopic details of the model.

The three-dimensional \(XY\) universality class is of particular interest, since the \(\lambda\)-transition of \(^4\)He is supposed to share this universality class. The experimental study of this transition provides by far the most precise experimental results for universal quantities like critical exponents and amplitude ratios. Thus this transition gives us a unique opportunity to test the ideas of the renormalization group and to benchmark theoretical methods. Most recent experiments with \(^4\)He were carried out during a Spacelab mission \[8,9\]. The condition of microgravity avoids the broadening of the transition due to the gravitational field and hence allows access to reduced temperatures down to \(t \approx 5 \times 10^{-10}\). The most recent analysis \[9\] of the Spacelab data gives \(\alpha = -0.0127(3)\) and \(A_+/A_- = 1.053(2)\) or

\[
R_\alpha = \frac{1 - A_+/A_-}{\alpha} = 4.154(22).
\]

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Note that $R_\alpha$ is much less correlated with the value of $\alpha$ than $A_+/A_-$ itself. This result can be compared with other experimental results $R_\alpha = 4.194(19)$ [10], $R_\alpha = 4.57(40)$ [11], $R_\alpha = 3.98(2)$, field theoretic estimates $R_\alpha = 4.433(77)$ [12], Monte Carlo simulations $R_\alpha = 4.20(5)$ [13] and high temperature expansions combined with the equation of state $R_\alpha = 4.3(2)$ [1]. Here we make no attempt to give a complete overview of theoretical results; we just try to give the most recent and we hope most accurate result for each of the methods.

Notice that some of these estimates of $R_\alpha$ are not consistent among themselves. This could be interpreted as a violation of universality; however we regard it as more likely that systematic errors are underestimated by some of the authors. Here we make an effort to keep errors, in particular the systematic error due to corrections to scaling, under control.

We studied the $\phi^4$ model on a cubic lattice with periodic boundary conditions in each of the directions. The lattice size is $L^3$, where $L$ is the linear extent of the lattice. The lattice spacing is set to $a = 1$. The classical Hamiltonian is given by

$$H = -\beta \sum_{\langle x,y \rangle} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x \left[ \phi_x^2 + \lambda(\phi_x^2 - 1)^2 \right],$$

(3)

where the field variable $\vec{\phi}_x$ is a vector with two real components. $\langle x, y \rangle$ denotes a pair of nearest neighbour sites. Note that in our convention, following reference [1], the inverse temperature $\beta$ is absorbed into the Hamiltonian but does not multiply its second term. The partition function is given by

$$Z(\beta, \lambda) = \int \mathcal{D}[\phi] \exp(-H(\beta, \lambda, \phi)), $$

(4)

where $\int \mathcal{D}[\phi]$ denotes the $2L^3$-dimensional integral over the field variables. In the limit $\lambda \to \infty$ the classical XY (plane rotator) model is recovered. Corrections to scaling amplitudes such as $c_\pm$ of equation (1) are functions of the parameter $\lambda$. It has been demonstrated that there exists a value $\lambda^*$ at which the amplitudes of the leading correction to scaling vanish. The most recent numerical estimate is $\lambda^* = 2.15(5)$ obtained in [1]. Previous estimates are $\lambda^* = 2.07(5)$ and $\lambda^* = 2.10(6)$ given in [7,14], respectively.

Here we shall analyse data for the specific heat and the energy density at $\lambda = 2.1$ and $\lambda = 2.2$. In [1] accurate estimates of the inverse critical temperature at various values of $\lambda$ are given. In the following we shall use

$$\beta_c = \begin{cases} 0.509 1503(3) [3] & \text{at } \lambda = 2.1, \\ 0.508 3355(3) [4] & \text{at } \lambda = 2.2. \end{cases}$$

(5)

The number in the parentheses gives the statistical error, while the number in brackets is an estimate of possible systematic errors.

The outline of the paper is the following. In the next section we define the energy and the specific heat for our lattice model. We summarize the predictions of the RG theory for the free energy density and the specific heat. In section 3 we present our numerical results. First we analyse the finite size behaviour of the energy density and the specific heat at the critical temperature. Then we discuss our results for the low and the high temperature phase. Finally an estimate for $R_\alpha$ is obtained by fitting these data to the expected power law behaviour.

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1 Reanalysis of the data of [11] in [9] assuming that the analytic background is indeed analytic at $T_c$. 

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2. Critical behaviour of the energy and the specific heat

The so called reduced free energy density is defined by

$$f(\beta, \lambda) = -\frac{1}{V} \ln Z(\beta, \lambda),$$

which is more convenient for our purposes than the usual $$-(T/V) \ln Z.$$

We define the energy density as

$$E = -\frac{\partial f}{\partial \beta} = \frac{1}{V} \sum \langle \phi_x \phi_y \rangle$$

and the specific heat as

$$C = -\frac{\partial^2 f}{\partial \beta^2} = \frac{1}{V} \left( \left\langle \left( \sum \langle \phi_x \phi_y \rangle \right)^2 \right\rangle - \left\langle \sum \langle \phi_x \phi_y \rangle \right\rangle^2 \right).$$

These definitions differ by factors $$-1$$ and $$\beta^2$$ from standard textbook definitions. Now, let us summarize the predictions of the RG theory for the free energy density. First, the free energy is split into a singular and a non-singular part

$$f = f_{ns} + f_s.$$ 

Let us first discuss the finite size scaling (FSS) behaviour of the free energy density for a system with periodic boundary conditions. To this end we briefly summarize the predictions of the RG theory. For a detailed discussion see e.g. [15,16]. The deviation of the non-singular part of the free energy density from its thermodynamic limit is exponentially small in $$L$$. The behaviour of the singular part is described by

$$f_s(u_t, u_h, \{u_i\}, L) = L^{-d} \Phi(L^{y_t} u_t, L^{y_h} u_h, \{L^{y_i} u_i\}),$$

where $$u_t \equiv u_1$$, $$u_h \equiv u_2$$, and $$\{u_i\}$$ with $$i \geq 3$$ are the scaling fields (which are analytic functions of the Hamiltonian parameters) associated with the reduced temperature $$t$$ ($$u_t \sim t$$), the magnetic field $$h$$ ($$u_h \sim h$$), and the irrelevant perturbations with RG exponents $$y_i < 0$$, respectively. $$d$$ is the dimension of the system; in our case $$d = 3$$. The RG exponent of the thermal scaling field is related to the critical exponent of the correlation length: $$y_t = 1/\nu$$. Furthermore the hyperscaling relation $$\alpha = 2 - d\nu = 2 - d/y_t$$ holds.

Let us consider the scaling of the energy density and the specific heat at the critical point $$u_t = 0$$ and $$u_h = 0$$. Taking the derivative with respect to $$\beta$$ and Taylor expanding in $$u_i$$ with $$i \geq 3$$ we get

$$E_s(L, \beta_c) = c_s L^{-d+y_t} (1 + d_1 L^{y_3} + d_2 L^{y_4} + \cdots)$$

and

$$C_s(L, \beta_c) = c_s L^{-d+2y_t} (1 + f_1 L^{y_3} + f_2 L^{y_4} + \cdots)$$

for the singular parts of the energy density and the specific heat, respectively.

The numerical values of the RG exponents are $$-y_3 = \omega = 0.785(20)$$ [1] and $$-y_4 = \omega_2 = 1.8(2)$$ [17,1]. The situation is complicated by the fact that $$y_5$$ is, within the numerical accuracy, degenerate with $$y_4$$ [17]. Furthermore, the breaking of

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rotational invariance by the lattice leads to corrections associated with an RG exponent 
$y_6 = -2.02(1)$ [18].

In the thermodynamic limit, for vanishing external field $h = 0$, the singular part of 
the free energy density behaves as

$$f_s = \tilde{a}_+ |t|^{2-\alpha} \left( 1 + c_{1,1,\pm} |t|^\Delta + c_{1,2,\pm} |t|^{2\Delta} + d_1 t + c_{2,1,\pm} |t|^{2\Delta} + \cdots \right)$$

with $\Delta = \nu \omega$ and $\Delta_2 = \nu \omega^2$. In the following we define the reduced temperature 
by $t = \beta - \beta_c$. Predictions for the singular parts of the energy density and the specific heat 
can be easily derived from equation (13) by taking the first and second derivatives with 
respect to $\beta$. One gets $e_s = a_+ |t|^{1-\alpha} (1 + \cdots)$ and $c_s = A_+ |t|^{-\alpha} (1 + \cdots)$ with

$$\frac{A_+}{A_-} = \frac{a_+}{a_-} = \frac{\tilde{a}_+}{\tilde{a}_-}.$$ (14)

3. The numerical results

Let us first sketch the strategy of our numerical analysis. We parametrize the non-singular 
part of the free energy by its Taylor expansion in the reduced temperature $t = \beta - \beta_c$:

$$f_{ns}(t) = f_{ns}(0) + e_{ns} t + \frac{1}{2} c_{ns} t^2 + \cdots.$$ (15)

In a first step of the analysis we determine $e_{ns}$ and $c_{ns}$ from the finite size behaviour of the 
energy density and the specific heat at the critical temperature. Then, in the analysis of 
the data for the thermodynamic limit at $\beta \neq \beta_c$, these estimates for $e_{ns}$ and $c_{ns}$ are used 
as input. In this respect, we essentially follow [13].

Note that the amplitudes of the leading correction to scaling are small at $\lambda = 2.1$ and $\lambda = 2.2$. Therefore we shall not take into account the leading correction to scaling in our 
fits. The systematic error introduced this way can be estimated by comparing the final 
results obtained for $\lambda = 2.1$ and $\lambda = 2.2$.

3.1. The energy density and the specific heat at the critical temperature

We analyse data for the energy density and the specific heat obtained on lattices of a linear 
size up to $L = 128$. The simulations are performed for some $\beta_s \approx \beta_c$. We have computed 
the Taylor coefficients of the energy density at $\beta_s$ up to second order. This allows us to 
compute the energy density and the specific heat in a sufficiently large neighbourhood of $\beta_s$.

Most of the data for $\lambda = 2.1$ were generated already for [7]. Some additional data, in 
particular data for $L = 128$, were generated more recently for [1]. In the case of $\lambda = 2.2$ 
the data for $L \leq 16$ and for $L = 128$ were generated for [1]. Here we have added new 
data for $L = 24, 32, 48$ and 64. In the Monte Carlo simulation a mixture of local and wall 
cluster [19] updates was used. For details we refer the reader to [7, 1].

First we have analysed the energy density at the central estimates of $\beta_c$ given in 
equation (5). In addition, to propagate the error of $\beta_c$, we have analysed the energy density at a slightly shifted value for $\beta_c$. We fitted our data using the ansatz

$$E = e_{ns} + e_s L^{-d+1/\nu}$$ (16)
without any correction term. We have performed these fits fixing \( \nu = 0.6717 \), which is the central estimate of [1], corresponding to \( \alpha = -0.0151 \). In addition we performed fits with slightly different values of \( \nu \) to determine the dependence of the result for \( c_{ns} \) on the input value of \( \nu \). For \( \nu = 0.6717 \), these fits lead to a \( \chi^2/\text{d.o.f.} \approx 1 \) starting from \( L_{\text{min}} = 6 \), where \( L_{\text{min}} \) is the minimal lattice size that has been included in the fit. Furthermore, the result for \( c_{ns} \) is very stable when \( L_{\text{min}} \) is increased. Also the statistical error of \( c_{ns} \) increases only slowly with increasing \( L_{\text{min}} \). Hence we regard the estimate of \( c_{ns} \) obtained from these fits as reliable. Being very conservative, we take our final result from fits with \( L_{\text{min}} = 24 \). Our results can be summarized as

\[
e_{ns} = 0.913213(5) + 20 \times (\beta - 0.5091503) + 5 \times 10^{-7} \times (1/\alpha + 1/0.0151)
\]  

(17)

for \( \lambda = 2.1 \) and

\[
e_{ns} = 0.913585(5) + 20 \times (\beta - 0.5083355) + 6 \times 10^{-7} \times (1/\alpha + 1/0.0151)
\]  

(18)

for \( \lambda = 2.2 \). For later use it is convenient to parametrize the dependence of the result on the input parameter \( \nu \) in terms of \( 1/\alpha \).

Next we have fitted the specific heat at \( \beta_c \) using the ansätze

\[
C = c_{ns} + c_\nu L^{-d+2/\nu}
\]

(19)

and

\[
C = c_{ns} + c_\nu L^{-d+2/\nu}(1 + f_2 L^{-\omega_2})
\]

(20)

with \( \nu = 0.6717 \) fixed. Fitting with ansatz (19) we get \( \chi^2/\text{d.o.f.} \approx 1 \) only for \( L_{\text{min}} > 16 \) for both values of \( \lambda \). Hence we also performed fits with ansatz (20) with \( \omega_2 = 1.8 \) fixed. Note that it is hopeless to add further correction terms like \( f_2 L^{-\omega_3} \) or \( f_4 L^{-\omega_4} \) to the ansatz. Since \( \omega_2 \approx \omega_3 \approx \omega_4 \), as discussed in the previous section, the term \( f_2 L^{-\omega_2} \) in equation (20) has to be viewed as an effective description of several corrections. To estimate the possible error due to this fact and also due to the numerical uncertainty of \( \omega_2 \) we have repeated the fits, now fixing \( \omega_2 = 2.0 \) instead of \( \omega_2 = 1.8 \). For both values of \( \omega_2 \) we get \( \chi^2/\text{d.o.f.} \approx 1 \) starting from \( L_{\text{min}} = 6 \). The results for \( c_{ns} \) obtained with \( \omega_2 = 1.8 \) fixed differ only little from those with \( \omega_2 = 2.0 \). In figure 1 we have plotted the results for \( c_{ns} \) obtained from the fits discussed above.

Guided by figure 1, we take, for both values of \( \lambda \), our final estimate of \( c_{ns} \) from the fit with ansatz (19) and \( L_{\text{min}} = 24 \). The error, which is indicated by dashed lines in figure 1, is chosen such that it covers the estimates from fits with ansatz (19) as well as with ansatz (20). The dependence of the final result on the input values of \( \beta_c \) and \( \nu \) is estimated by redoing the fit with ansatz (19) and \( L_{\text{min}} = 24 \) for values of \( \nu \) and \( \beta_c \) slightly different to those chosen above. As result we obtain

\[
c_{ns} = 157.9(5) + 147000 \times (\beta - 0.5091503) - 2.1 \times (1/\alpha + 1/0.0151)
\]

(21)

for \( \lambda = 2.1 \) and

\[
c_{ns} = 155.6(4) + 121000 \times (\beta - 0.5083355) - 2.1 \times (1/\alpha + 1/0.0151)
\]

(22)

for \( \lambda = 2.2 \).

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Figure 1. The non-singular part of the specific heat $c_{ns}$ obtained from numerical data at $\beta_c$ as a function of the smallest lattice size $L_{\text{min}}$ that has been included in the fit. We have used either an ansatz without any correction to scaling (19) or an ansatz with subleading corrections to scaling (20) with an exponent $\omega_2 = 1.8$. For details see the text.

3.2. The energy density in the thermodynamic limit

The simulations in the high temperature phase were already discussed in [1]. In the high temperature phase we expect the observables to converge exponentially fast to the thermodynamic limit as $L \to \infty$. Throughout we have used $L > 10\xi$ in these simulations.
Figure 2. The energy density $E$ at $\lambda = 2.1$ and $\beta = 0.51$ is plotted as a function of $L^{-3}$, where $L$ is the linear lattice size. The circles give our Monte Carlo results for the lattice sizes $L = 128, 144, 192, 256$ and $288$. The triangle gives the result of the extrapolation to $L = \infty$ with ansatz (23). In the fit $L = 128$ had been excluded.

In particular for our largest correlation length $\xi \approx 30$ we used $L = 350$. Hence within our numerical accuracy, the results should coincide with the thermodynamic limit.

In the low temperature phase, the breaking of the continuous $U(1)$ symmetry leads to a Goldstone mode. As a result, leading corrections to the thermodynamic limit of the energy density are $O(L^{-3})$ [20, 21]. We fitted our data for the energy density with the ansatz

$$E(L) = E(\infty) + cL^{-3}. \quad (23)$$

Typically, the difference $E(\infty) - E(L_{\text{max}})$ of the fit result for the thermodynamic limit and the result for the largest lattice size $L_{\text{max}}$ that we have simulated are of a similar size to the statistical error of $E(L_{\text{max}})$ and $E(\infty)$. Therefore we are confident that the quoted error, which is the statistical error of the result of the fit with ansatz (23), is reliable. For illustration we have plotted in figure 2 the Monte Carlo results for the energy density $E$ at $\lambda = 2.1$ and $\beta = 0.51$ as a function of $L^{-3}$. Our final results for the thermodynamic limit of the energy density are summarized in table 1. In addition we give the second-moment correlation length $\xi_{\text{2nd}}$ in the high temperature phase.

We have also measured the specific heat. However the result for $R_\alpha$ obtained from these data is consistent with but less precise than that obtained from the energy density. Therefore we skip the discussion of the specific heat data.

First we have fitted our data for the energy density with the ansatz

$$E = e_{\text{ns}} + c_{\text{ns}}(\beta - \beta_c) + a_\pm|\beta - \beta_c|^{1-\alpha}. \quad (24)$$

In these fits, we take $\alpha$, $\beta_c$ and the corresponding values of $e_{\text{ns}}$, equations (17), (18), and $c_{\text{ns}}$, equations (21), (22), as input.
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Table 1. Results for the energy density $E$ of the $\phi^4$ model at $\lambda = 2.1$ and $\lambda = 2.2$ in the thermodynamic limit for various values of the inverse temperature $\beta$. In addition we give the second-moment correlation length $\xi_{2nd}$ in the high temperature phase.

| $\lambda$ | $\beta$ | $\xi_{2nd}$ | $E$     |
|-----------|--------|-------------|---------|
| 2.1       | 0.503  | 8.042       | 0.856373(7) |
| 2.1       | 0.505  | 10.482      | 0.871351(8) |
| 2.1       | 0.506  | 12.626      | 0.879580(6) |
| 2.1       | 0.507  | 16.318      | 0.888476(7) |
| 2.1       | 0.5075 | 19.498      | 0.893283(9) |
| 2.1       | 0.508  | 24.845      | 0.898418(6) |
| 2.1       | 0.5083 | 30.453      | 0.901727(4) |
| 2.1       | 0.51   |             | 0.931674(14) |
| 2.1       | 0.5105 |             | 0.941232(16) |
| 2.1       | 0.511  |             | 0.950382(13) |
| 2.1       | 0.512  |             | 0.967852(11) |
| 2.1       | 0.513  |             | 0.984474(10) |
| 2.1       | 0.515  |             | 1.016005(30) |
| 2.2       | 0.501  | 7.1723      | 0.849150(4)  |
| 2.2       | 0.5035 | 9.502       | 0.866864(5)  |
| 2.2       | 0.5055 | 13.610      | 0.882972(5)  |
| 2.2       | 0.5067 | 19.710      | 0.894014(6)  |
| 2.2       | 0.50748| 30.475      | 0.902171(4)  |
| 2.2       | 0.5095 |             | 0.937817(19) |
| 2.2       | 0.51   |             | 0.947000(19) |
| 2.2       | 0.511  |             | 0.964370(17) |
| 2.2       | 0.512  |             | 0.980920(19) |

It turns out that in the case of $\lambda = 2.1$, fits that include $|\beta - \beta_c| \leq 0.005$ have a large $\chi^2$/d.o.f. To understand this problem we resorted to a simpler analysis of the data. We took pairs of inverse temperatures such that $\beta_c - \beta_1 \approx \beta_2 - \beta_1$. These two values are sufficient for determining the parameters $a_+$ and $a_-$ of the ansatz (24). In figure 3 we give the results for $R_\alpha$ obtained in this way as a function of $(\beta_2 - \beta_1)/2$. We see that the estimate of $R_\alpha$ is roughly linear in $\beta_2 - \beta_1$. A linear extrapolation to $\beta_2 - \beta_1 = 0$ suggests a value of $R_\alpha$ that is slightly larger than 4.

Motivated by this observation, we performed fits with the ansatz

$$E = c_{ns} + c_{ns}(\beta - \beta_c) + a\pm|\beta - \beta_c|^{1-\alpha} + d(\beta - \beta_c)^2,$$

(25)

where we have added a further term to the Taylor expansion of the analytic part of the energy density. Note that the first analytic correction to the singular part comes with a very similar exponent: $2 - \alpha$. Hence the fit parameter $d$ will provide only an effective amplitude for the combination of the two terms. Note that also the exponent of subleading corrections $1 - \alpha + \Delta_2$ is only slightly larger than 2. We also tried to explicitly take into account these terms in the fit. This leads however to very large errors for the coefficients.

Using ansatz (25) we get fits with a $\chi^2$/d.o.f. smaller than one for the interval $0.506 \leq \beta \leq 0.512$ and $0.5055 \leq \beta \leq 0.511$ for $\lambda = 2.1$ and $\lambda = 2.2$, respectively. Using

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Figure 3. Estimate of $R_\alpha$ obtained from two values of the inverse temperature $\beta_1$ and $\beta_2$, using the ansatz (24). Only results for $\lambda = 2.1$ are given. Two errors are displayed: the smaller one is that due to the statistical error of the energy density at $\beta_1$ and $\beta_2$; the larger one is due to the uncertainty of $c_{\text{ns}}, e_{\text{ns}}$ and $\beta_c$. The dotted line is only to guide the eye.

In order to check for the effect of corrections to the ansatz (25) discussed above, we have repeated the fits using values of $\beta$ that are further off from $\beta_c$. In particular, fitting the data for $\beta = 0.503, 0.505, 0.506, 0.512, 0.513, 0.515$ in the case of $\lambda = 2.1$ we obtain $R_\alpha = 4.006(3)$ and fitting the data for $\beta = 0.501, 0.5035, 0.5055, 0.511, 0.512$ in the case of $\lambda = 2.2$ we obtain $R_\alpha = 3.988(2)$. Note that the average of $|\beta - \beta_c|$ for this second set of fits is more than twice as large as for the first set of fits.

Next we computed the error of $R_\alpha$ due to the uncertainty of the input values of $c_{\text{ns}}, e_{\text{ns}}$ and $\beta_c$. To this end, we repeated the fits using the central values of $c_{\text{ns}}, e_{\text{ns}}$ and $\beta_c$ shifted by the error estimate. Summing the errors of $R_\alpha$ due these input values we get a little less than 0.02 for both values of $\lambda$.

Finally, we have also repeated the fits for $\alpha \neq 0.0151$ to obtain the dependence of our numerical estimate of $R_\alpha$ on $\alpha$.

Summing all errors discussed above, we arrive at the final estimate

$$R_\alpha = 4.01(5) - 8 \times (\alpha + 0.0151).$$

Notice that the dependence on $\alpha$ is rather small; e.g. inserting the estimate $\alpha = -0.0127$ of [9] we get $R_\alpha = 3.99$. 

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4. Conclusions and comparison with the literature

We have studied the universal amplitude ratio $A_+/A_-$ of the specific heat in the three-dimensional $XY$ universality class. Since $|\alpha|$ is rather small, it is difficult to disentangle the singular and the non-singular part of the specific heat or the energy density. This problem holds for numerical data obtained from Monte Carlo simulations of lattice models as well as for experimental data.

While in [13] the standard $XY$ model was simulated we have studied the improved $\phi^4$ model, allowing us to ignore leading corrections to scaling in the analysis of the data. Given the problem discussed above, this is an important advance.

In our analysis we have combined information from the finite size scaling behaviour at the transition [1,7] with precise results for the thermodynamic limit in the low and the high temperature phase. Reaching correlation lengths up to $\xi_{2nd} \approx 30$ subleading corrections to scaling are under control.

We made an effort to take carefully into account various sources of systematic error. Pessimistically we have summed these errors to arrive at our final estimate $R_\alpha = (1 - A_+/A_-)/\alpha = 4.01(5)$.

Our estimate for $R_\alpha$ is significantly smaller than most theoretical and experimental results. There is only good agreement with the experimental result $R_\alpha = 3.98(2)$ (see footnote 1).

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