# $A_+/A_-$, $\alpha$, $\nu$, and $f_s\xi^3$ from 3D Ising energy and specific heat



1998 J. Phys. A: Math. Gen. 31 6157

(http://iopscience.iop.org/0305-4470/31/29/007)

J. Phys. A: Math. Gen. **31** (1998) 6157–6166. Printed in the UK PII: S0305-4470(98)84766-5

# $A_+/A_-$, $\alpha$, $\nu$, and $f_s\xi^3$ from 3D Ising energy and specific heat

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Received 4 June 1997, in final form 27 February 1998

**Abstract.** We analyse Monte Carlo data for the energy and specific heat at and close to the critical point of the 3D cubic Ising model. From the finite-size scaling of the energy $E$ and the specific heat $C$ at criticality we obtain the estimate $\nu = 0.6308(10)$. Furthermore, one obtains precise estimates for the 'backgrounds' (nonsingular parts) $E_{\rm ns}$ and $C_{\rm ns}$. Fitting solely off-critical energy estimates to a scaling law, we find, depending on the choice of the reduced temperature, either $A_+/A_- = 0.550(12)$ and $\alpha = 0.1115(37)$, or $A_+/A_- = 0.567(16)$ and $\alpha = 0.1047(48)$. Including information from the data at $T_c$, we obtain the estimate $A_+/A_- = 0.560(10)$. We also determine the universal combination $f_s\xi^3$ in both phases.

## 1. Introduction

The universal amplitude ratio $A_+/A_-$ of the 3D Ising universality class (for a precise definition see equation (6) below) still seems subject to some uncertainty. For a general discussion of the difficulties one encounters when trying to estimate $A_+/A_-$ from high and low temperature expansions see [1]. A compilation of some results in the literature will be given in section 4. For a general introduction to universal critical-point amplitudes see, e.g. [2].

Here we present a calculation of $A_+/A_-$ based on Monte Carlo (MC) data for the energy of the 3D Ising model. Furthermore, we obtain fairly precise estimates of other quantities, such as the exponents $\nu$ and $\alpha$, nonsingular parts of energy and specific heat, and of the universal combination $f_s\xi^3$ on both sides of the transition.

Consider the 3D Ising model on the simple cubic lattice of size $L \times L \times L$, with periodic boundary conditions. The Hamiltonian is

$$H = -\sum_{\langle x,y\rangle} s_x s_y \qquad s_x = \pm 1. \tag{1}$$

The sum in equation (1) is over all (unordered) nearest-neighbour pairs of sites in the lattice. The partition function is

$$Z = \sum_{\{s\}} \exp(-\beta H). \tag{2}$$

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0305-4470/98/296157+10$19.50  

Here, the summation is over all possible configurations of the Ising spins. The pair interaction is normalized such that $\beta = 1/(k_B T)$, where $k_B$ denotes Boltzmann's constant, and $T$ is the temperature.

At a critical coupling $\beta_c = 0.221\,6544(6)$ [3] the model undergoes a second-order phase transition. For $\beta > \beta_c$, the system shows spontaneous breaking of reflection symmetry.

The free energy density (free energy per link) is defined by

$$f = -\frac{1}{3L^3} \ln Z. \tag{3}$$

We define the energy (per link) as the derivative of $f$ with respect to $\beta$,

$$E = -\frac{\mathrm{d}}{\mathrm{d}\beta} f = -\frac{1}{3L^3} \langle H \rangle. \tag{4}$$

The specific heat is defined as the derivative of $E$ with respect to $\beta$,

$$C = \frac{\mathrm{d}}{\mathrm{d}\beta} E = \frac{1}{3L^3} (\langle H^2 \rangle - \langle H \rangle^2). \tag{5}$$

Note that choosing other definitions, such as putting a minus sign in equation (4) or substituting a $\mathrm{d}/\mathrm{d}T$ instead of the $\mathrm{d}/\mathrm{d}\beta$ in equation (5) leads to trivial factors and/or signs in the definitions and results to be stated below.

The specific heat is singular at the critical point. Close to $\beta_c$ it is expected to behave like

$$C \simeq C_{\mathrm{ns}} + C_{\mathrm{s}} \tag{6}$$

where $C_{\mathrm{ns}}$ is an analytic function of $\beta$ at $\beta_c$. The singular part is

$$C_{\mathrm{s}} \simeq A_{\pm} |t|^{-\alpha} \tag{7}$$

where

$$t = 1 - \frac{\beta}{\beta_c} \tag{8}$$

is the reduced temperature. $A_+$ and $A_-$ denote the amplitudes of the singular part in the symmetric ($t > 0$) and broken ($t < 0$) phase, respectively. $\alpha$ is the specific heat exponent. The singularity of the specific heat implies a nonanalytic behaviour of the energy $E$ and the free energy density $f$. Some details will be given in section 2.

## 2. Scaling and finite-size scaling

For a general introduction to finite-size scaling theory, see e.g. [4]. In order to discuss the nonanalytic behaviour of the free energy density it is useful to split it into an analytic (nonsingular) and a singular part,

$$f = f_{\mathrm{ns}} + f_{\mathrm{s}}. \tag{9}$$

Renormalization group arguments lead to the following finite-size scaling ansatz for the singular part of the free energy density for lattices with periodic boundary conditions [5],

$$f_{\mathrm{s}} \xi^d \simeq g(\xi/L) \tag{10}$$

where $f_{\mathrm{s}}$ is taken in the finite volume, while $\xi$ is the correlation length defined in the thermodynamic limit. $g(\xi/L)$ is a universal function. In the following we discuss the two extremal cases of the thermodynamic limit and the finite-size scaling exactly at the critical point.

The thermodynamic limit is characterized by $\xi/L = 0$. Inserting the scaling ansatz $\xi \sim t^{-\nu}$ into equation (10) for $\xi/L = 0$ we obtain

$$f_s \sim t^{d\nu}. \tag{11}$$

By differentiation with respect to $\beta$ we arrive at

$$E_s \sim t^{d\nu-1} \tag{12}$$

and

$$C_s \sim t^{d\nu-2}. \tag{13}$$

The last equation implies the so-called hyperscaling relation $\alpha = 2 - d\nu$.

In order to discuss finite-size scaling at the critical point it is useful to reparametrize equation (10) as

$$f_s L^d \simeq h(L/\xi) \tag{14}$$

with $h(L/\xi) = (L/\xi)^d g(\xi/L)$. Inserting the scaling law $\xi \sim t^{-\nu}$ we obtain

$$f_s \simeq L^{-d}\tilde{h}(L^{1/\nu}t) \tag{15}$$

and, by differentiation with respect to $\beta$,

$$E_s \sim L^{-d+1/\nu}\tilde{h}'(L^{1/\nu}t) \tag{16}$$

and

$$C_s \sim L^{-d+2/\nu}\tilde{h}''(L^{1/\nu}t). \tag{17}$$

For the critical temperature $t = 0$ this means

$$E_s \sim L^{-d+1/\nu} \tag{18}$$

and

$$C_s \sim L^{-d+2/\nu}. \tag{19}$$

In our numerical study we approximated the nonsingular part of the free energy density by its Taylor expansion, truncated at second order,

$$f_{ns} \simeq F_{ns} - E_{ns}(\beta - \beta_c) - \tfrac{1}{2}C_{ns}(\beta - \beta_c)^2 \tag{20}$$

where $F_{ns}$, $E_{ns}$ and $C_{ns}$ are the nonsingular parts of the free energy density, the energy density and the specific heat at the critical point, respectively.

## 3. MC simulations

### *3.1. Simulations at $\beta_c$*

We simulated the model at $\beta_c = 0.221\,6544$ on lattices of size $L = 12$ up to $L = 112$. For the simulation we employed the single-cluster algorithm. The updating between two measurements consisted of a number of clusters, ranging between 5 and 50, and a single Metropolis sweep. The total number of measurements was several million for the smaller lattice and some hundred thousands for the larger systems.

We measured the energy $E$, the specific heat $C$ and the derivative of $C$ with respect to the inverse temperature $\beta$. Our results for $E$ and $C$ are summarized in table 1.

We fitted our data for the energy and the specific heat according to the ansatz

$$E = E_{ns} + \text{constant}_E L^{-d+1/\nu} \tag{21}$$

**Table 1.** Results for the energy $E$ and the the specific heat $C$ at $\beta_c = 0.221\,6544$ for various lattice sizes $L$.

| $L$ | $E$ | $C$ |
|---|---|---|
| 12 | 0.352 212(10) | 11.0572(24) |
| 16 | 0.344 859(16) | 12.2103(58) |
| 20 | 0.340 931(7) | 13.1588(47) |
| 24 | 0.338 489(12) | 13.9138(95) |
| 28 | 0.336 873(6) | 14.5920(55) |
| 32 | 0.335 721(6) | 15.1921(74) |
| 36 | 0.334 882(6) | 15.7199(84) |
| 40 | 0.334 233(7) | 16.222(19) |
| 44 | 0.333 735(6) | 16.652(11) |
| 48 | 0.333 302(10) | 17.075(25) |
| 56 | 0.332 701(8) | 17.800(21) |
| 64 | 0.332 286(9) | 18.483(30) |
| 72 | 0.331 954(9) | 19.059(41) |
| 80 | 0.331 720(7) | 19.617(32) |
| 96 | 0.331 365(8) | 20.517(65) |
| 112 | 0.331 145(8) | 21.439(80) |

**Table 2.** Results of fits of the energy $E$ and the the specific heat $C$ at $\beta_c = 0.221\,6544$. The upper part gives results from energy data only, the following three rows state results from specific heat data only, while the lower part refers to fits where both sets of data were combined. Only data of simulations with lattice size greater than or equal to $L_{\min}$ were used for the fits. $X$ denotes $\chi^2$ per degree of freedom.

| Data | $L_{\min}$ | $X$ | $\nu$ | Constant$_E$ | $E_{\rm ns}$ | Constant$_C$ | $C_{\rm ns}$ |
|---|---|---|---|---|---|---|---|
| Energy | 12 | 1.04 | 0.6280(5) | 0.7276(25) | 0.330 190(7) | | |
| data | 16 | 1.13 | 0.6282(10) | 0.729(5) | 0.330 192(9) | | |
| only | 20 | 0.86 | 0.6296(12) | 0.737(7) | 0.330 200(9) | | |
| Specific | 12 | 1.42 | 0.6380(7) | | | 20.9(8) | −18.2(9) |
| heat data | 16 | 1.35 | 0.6365(13) | | | 19.3(1.2) | −16.4(1.4) |
| only | 20 | 0.45 | 0.6329(16) | | | 16.1(1.3) | −12.9(1.4) |
| Both | 12 | 5.6 | 0.6316(4) | 0.7440(20) | 0.330 229(5) | 15.32(30) | −12.13(33) |
| data | 16 | 2.25 | 0.6315(8) | 0.7460(40) | 0.330 218(7) | 15.15(54) | −11.83(61) |
| combined | 20 | 0.75 | 0.6308(10) | 0.7431(52) | 0.330 209(8) | 14.58(66) | −11.12(76) |

and

$$C = C_{\rm ns} + \text{constant}_C L^{-d+2/\nu} \tag{22}$$

that are motivated by equations (18) and (19), respectively. The results are summarized in table 2. The $\chi^2$ per degree of freedom becomes smaller than one if only lattices with $L \geqslant 20$ are included in the fit.

One observes that the result for $\nu$ obtained from the energy is smaller than that from fitting the specific heat. However, when discarding data from small $L$ the estimate of $\nu$ from the energy increases, while that from the specific heat decreases.

Next we fitted the data for the energy and the specific heat simultaneously. We checked that the cross-correlation of the two quantities is small compared with the geometric mean of the variances of the two quantities. Therefore it is justified to treat, for simplicity, the

**Table 3.** A collection of results for the exponents $\nu$ and $\alpha$ obtained with various methods. The abbreviations for the methods used are explained in the text.

| Reference | Method | $\nu$ | $\alpha$ |
|---|---|---|---|
| [6] | $\epsilon$-expansion | 0.6310(15) | 0.1100(45) |
| [6] | 3D, FT | 0.6300(15) | 0.1100(45) |
| [9] | 3D, FT | 0.630 | |
| [12] | HT, $\phi^4$ | 0.6300(15) | |
| [11] | HT | | 0.101(4) |
| [13] | HT | | 0.104(4) |
| [7] | MC | 0.6301(8) | |
| [8] | CAM | | 0.108(5) |
| [10] | FSS, exact | 0.629(2) | |

data as independent. When all data are included into the fit the $\chi^2$ per degree of freedom becomes unacceptably large. Again discarding the $L = 12$ and $L = 16$ data, the fits become very good. It is interesting to note that the value for $\nu$ changes only slightly when $L = 12$ and 16 are discarded from the fit.

In order to check the dependence of our result on the value of the critical coupling, we repeated the fit for $\beta = 0.221\,6538$ and $\beta = 0.221\,655$. The values for the energy and the specific heat at these $\beta$-values were obtained from first-order Taylor expansion and the numerically determined values of the derivatives. Taking into account the error induced by the uncertainty of $\beta_c$ we arrive at the final estimates $E_{\rm ns} = 0.330\,209(14)$, $C_{\rm ns} = -11.1(8)$ and $\nu = 0.6308(10)$ obtained from the combined energy and specific heat fit with $L \geqslant 20$. Here only statistical errors are given. It is difficult to quantify systematic errors owing to corrections to scaling. We tried to use an ansatz that includes a leading correction to scaling term

$$E_{\rm s} \sim L^{-d+1/\nu}(1 + cL^{-\omega}) \tag{23}$$

with the correction to scaling exponent $\omega = 0.81(5)$ [3, 6, 9, 12, 7]. It turned out that the amplitude of the correction to the scaling term was consistent with zero within error bars. The estimate of $\nu$ was $\nu = 0.631(4)$ when all data for the energy and the specific heat were included in the fit.

A discussion of results for critical exponents obtained from various methods can be found in section 7 of [7]. For the convenience of the reader we summarize some of the more recent results for the exponents $\nu$ and $\alpha$ in table 3. These results were obtained with $\epsilon$-expansion, field theoretic methods applied to 3D $\phi^4$ theory (3D, FT), high-temperature expansions (HT) of the 3D Ising model and the $\phi^4$ theory, the coherent-anomaly method applied to the 3D Ising model (CAM) and finite-size scaling (FSS) of a 2D Ising Hamiltonian system which is computed exactly on lattices of size up to $5^2$ (while the time direction is continuous as well as infinite).

All estimates are nicely consistent among each other except the one obtained by Guttmann and Enting [11]. Their result for $\alpha$ is by about twice the cited uncertainty 0.004 smaller than $\alpha = 0.110$ or $\nu = 0.630$ by hyperscaling which is roughly the average of the other results given.

Since the estimate of $\nu$ obtained from the fit without corrections to scaling is in good agreement with recent results given in the literature, we also regard the estimates for $E_{\rm ns}$ and $C_{\rm ns}$, which will be used in the following, as reliable.

A more detailed account of corrections to scaling is given in sections 5.1 and 5.2 of

[7]. The data set of [7] contains high statistics runs of small lattices and should hence be more suitable than our data to detect corrections to scaling.

It is interesting to note that the leading correction to scaling amplitudes, $b_1$ (energy) and $r_1$ (specific heat) in the notation of [7], are consistent with zero within the error bars.

The final results for $E_{\rm ns}$ and $C_{\rm ns}$ of [7] are consistent with ours. However, in this case our statistical errors are considerably smaller. Here we benefit from the larger lattice sizes available ($L_{\rm max} = 112$ in contrast to $L_{\rm max} = 40$ of [7]).

### *3.2. Simulations at $\beta \neq \beta_c$*

Next we simulated the model at temperatures below and above the critical temperature, such that results for the thermodynamic limit could be obtained. The resulting MC estimates for $E$ are fitted to

$$E \simeq E_{\rm ns} - C_{\rm ns}\beta_c t \mp A_{\pm}\beta_c \frac{|t|^{1-\alpha}}{1-\alpha} \tag{24}$$

which is obtained by integration of equation (6). For the simulations in the symmetric phase and for part of the simulations in the broken phase we used the single cluster algorithm [14] combined with a standard local Metropolis update. A typical mixture was 20 cluster updates plus a single Metropolis sweep, followed by a measurement of observables. The total number of measurements was typically of order a few hundred thousand up to two million. Part of the results for the broken phase were obtained in the course of another project [15], using a demon program coded in multispin fashion. For details of these simulations we refer to [15].

Our results for $E$ are displayed in table 4. The $\beta$-values were chosen in the range 0.218 909–0.224. The corresponding reduced temperature covers the interval from 0.0124 to $-0.011$. The typical lattice sizes were 96 and 128. We convinced ourselves that we always reached the thermodynamic limit within the numerical precision. In the table we marked those values that were discarded because of finite-size effects by an 'F'. Data that were excluded because of a too large a distance from criticality are marked with a 'T' (see below).

We then made two types of fits. We first fixed $\beta_c$ and $\alpha$, and fitted $E_{\rm ns}$, $C_{\rm ns}$, $A_+$, and $A_-$. Then we only fixed $\beta_c$ and fitted all the other parameters in equation (24). In both cases, we used in addition to the reduced temperature $t$ an alternative definition,

$$t' = \frac{\beta_c}{\beta} - 1. \tag{25}$$

Comparing the fit results from the two definitions should give us an estimate of systematic effects that stem, e.g. from the inclusion of data that have too large a $t$ or the neglection of subleading terms in equation (24). The results for the fit parameters are summarized in table 5.

We first started taking all the data of table 4. However, it turned out that in order to have fits with a reasonable level of confidence, we had to discard the data marked with a 'T'. The fits with the remaining data (the results of which are quoted in table 5) had a $\chi^2$ per degree of freedom of 0.9–1.2.

There is a systematic difference of the fits with the two different definitions of the reduced temperature. In the case of the fits with fixed $\alpha$ we could further reduce the data to include only results closer to criticality. This moved the estimates slightly, however, it did not diminish the systematic difference between the $t$ and $t'$ fits. We therefore conclude

**Table 4.** MC results for the energy of the 3D off-critical Ising model. A 'T' in the last column means that the corresponding data is not used for the fits because of its too large reduced temperature. Exclusion of the fits because of finite-size effects is indicated by an 'F'.

| $\beta$ | $E$ | $L$ | |
|---|---|---|---|
| 0.218 9088 | 0.311 775(5) | 96 | T |
| 0.219 31 | 0.313 849(14) | 80 | T |
| 0.219 7088 | 0.315 949(6) | 96 | |
| 0.220 2 | 0.318 742(11) | 100 | |
| 0.220 4 | 0.319 958(6) | 96 | |
| 0.220 5 | 0.320 587(9) | 128 | |
| 0.220 5 | 0.320 592(9) | 96 | |
| 0.220 6 | 0.321 230(11) | 128 | |
| 0.220 6 | 0.321 220(8) | 96 | |
| 0.220 7 | 0.321 887(9) | 128 | |
| 0.220 7 | 0.321 900(8) | 96 | |
| 0.220 8 | 0.322 581(9) | 128 | |
| 0.220 8 | 0.322 593(9) | 96 | |
| 0.220 9 | 0.323 280(5) | 128 | |
| 0.220 9 | 0.323 301(8) | 96 | F |
| 0.221 0 | 0.323 995(10) | 128 | |
| 0.221 0 | 0.324 040(9) | 96 | F |
| | | | |
| 0.222 0 | 0.340 001(12) | 128 | |
| 0.222 0 | 0.340 001(34) | 96 | |
| 0.222 1 | 0.342 368(19) | 96 | |
| 0.222 2 | 0.344 592(35) | 96 | |
| 0.222 4 | 0.348 911(35) | 96 | |
| 0.222 6 | 0.353 134(36) | 96 | |
| 0.222 8 | 0.357 057(36) | 96 | |
| 0.222 9 | 0.358 935(47) | 64 | |
| 0.223 0 | 0.360 972(31) | 96 | |
| 0.223 4 | 0.368 280(28) | 96 | T |
| 0.223 6 | 0.371 725(27) | 96 | T |
| 0.223 8 | 0.375 248(27) | 96 | T |
| 0.224 0 | 0.378 615(26) | 96 | T |

that in order to cure this problem the most likely correction terms should be added in the ansatz equation (24). To this end, one would probably need more precise data.

The slight mismatch of the result for $E_{\rm ns}$ obtained in this section with the result obtained from finite-size scaling at the critical point should be attributed to such corrections to scaling and not to a failure of the theoretical prediction.

Using the results for $E_{\rm ns}$, $C_{\rm ns}$ and $\nu$ obtained at the critical point one can compute the scaling amplitude from a single energy value, just by solving equation (24) with respect to $A_+$ or $A_-$. The results are given in table 6.

The main sources of error in the amplitudes $A_+$ and $A_-$ computed this way are induced by the errors of $C_{\rm ns}$ and $\nu$. However, when taking the ratio $A_+/A_-$ from amplitudes computed at about the same distance from $\beta_c$ the dependence on $\nu$ completely cancels, and also the error by $C_{\rm ns}$ partially cancels. When taking the amplitudes obtained from the $\beta$-values closest to $\beta_c$ we obtain $A_+/A_- = 0.560(10)$, which is consistent with the result that was obtained using only data with $\beta \neq \beta_c$.

Let us now make a comparison with a few results of the literature. Estimates from $\epsilon$-expansion, field theoretic calculations in $D = 3$, high-temperature expansions and from

**Table 5.** Results for the fit parameters of equation (24). An 'f' in the first column means that the corresponding parameter was kept fixed to the quoted value. $t$ and $t'$ indicate the definition of reduced temperature that was employed in the fit.

| $\alpha$ | Type | $A_+$ | $A_-$ | $A_+/A_-$ | $E_{\rm ns}$ | $C_{\rm ns}$ |
|---|---|---|---|---|---|---|
| 0.100 f | $t$ | 11.194(56) | 19.068(42) | 0.5871(16) | 0.330 37(1) | −12.561(96) |
| | $t'$ | 11.147(51) | 19.132(41) | 0.5826(15) | 0.330 33(1) | −12.544(88) |
| 0.104 f | $t$ | 10.374(52) | 18.076(39) | 0.5739(17) | 0.330 34(1) | −11.549(91) |
| | $t'$ | 10.329(47) | 18.140(38) | 0.5694(15) | 0.220 30(1) | −11.545(85) |
| 0.108 f | $t$ | 9.625(49) | 17.160(37) | 0.5609(17) | 0.330 31(1) | −10.613(89) |
| | $t'$ | 9.582(45) | 17.224(36) | 0.5563(15) | 0.330 27(1) | −10.601(88) |
| 0.112 f | $t$ | 8.940(47) | 16.311(34) | 0.5481(18) | 0.330 28(1) | −9.743(85) |
| | $t'$ | 8.900(42) | 16.375(33) | 0.5435(15) | 0.330 24(1) | −9.733(78) |
| 0.1115(37) | $t$ | 9.03(63) | 16.42(77) | 0.550(12) | 0.330 29(3) | −9.86(80) |
| 0.1047(48) | $t'$ | 10.19(96) | 17.97(1.17) | 0.567(16) | 0.330 30(4) | −11.37(1.17) |

**Table 6.** Estimates for the amplitudes $A_\pm$ based on the estimates $E_{\rm ns} = 0.330\,209(14)$, $C_{\rm ns} = 11.1(8)$ and $\nu = 0.6308(10)$. The estimates are obtained by solving equation (24) with respect to $A_+$ or $A_-$ a fixed $\beta$, assuming hyperscaling $\alpha = 2 - d\nu$. The dominant sources of error in the resulting amplitudes are the errors of $C_{\rm ns}$ and $\nu$. These errors are displayed in the first and second parentheses respectively.

| $\beta$ | $A_+$ | $\beta$ | $A_-$ |
|---|---|---|---|
| 0.2204 | 9.86(41)(18) | 0.2220 | 17.55(36)(46) |
| 0.2205 | 9.85(40)(19) | 0.2221 | 17.56(37)(39) |
| 0.2206 | 9.85(40)(19) | 0.2222 | 17.52(37)(37) |
| 0.2207 | 9.84(39)(19) | 0.2224 | 17.50(39)(36) |
| 0.2208 | 9.82(39)(20) | 0.2226 | 17.53(40)(35) |
| 0.2209 | 9.82(39)(20) | 0.2228 | 17.49(41)(34) |
| 0.2210 | 9.82(38)(20) | | |

experiments are given in [16]. For the readers convenience, we reproduce part of that table in our table 7 and complete it with our present estimates. Apparently, our estimates are larger than those cited in the table. However, our most accurate estimate MC, (c) is consistent within error bars with the most recent result form $\epsilon$-expansion [16] and the results from renormalized perturbation theory in three dimensions [18, 16]. We think that the disagreement with the estimate based on high- and low-temperature expansion is most likely due to an underestimation of the error in [1].

## 4. The universal constant $f_{\rm s}\xi^d$

In this section we try to extract the numerical value of $f_{\rm s}\xi^d$ in both phases of the model. The values for the second moment correlation length $\xi_{\rm 2nd}$ are taken from [19].

The estimates for $f_{\rm s}$ at given $\beta$-values were obtained in the following way. We took $E - E_{\rm ns} - C_{\rm ns}(\beta - \beta_c)$ as an approximation of the singular part of the energy. The constants $E_{\rm ns}$ and $C_{\rm ns}$ were taken from the combined energy and specific heat fit at the critical point. Then we computed $f_{\rm s}$ as the integral over $\beta$ of the singular part of the energy. We interpolated the singular part of the energy for $\beta$-values not simulated with the scaling ansatz, where we use $\nu = 0.6308$ and the amplitude was computed from the closest $\beta$-value

**Table 7.** Amplitude ratio estimates taken from the literature and from this work. The estimate (a) and (b) are the fit results quoted in table 5, and discussed in section 2.2. Estimate (a) was obtained by including also information from the data at the critical point, cf the discussion at the end of section 2.2. Some estimates from experiments are 0.56(2) (binary mixtures), 0.49–0.53 (liquid–vapour systems), and 0.49–0.54 (magnetic systems), see [2].

| Method | $A_+/A_-$ | Reference | Year |
|---|---|---|---|
| $\epsilon$-expansion | 0.524(10) | [17] | 85/86 |
| $\epsilon$-expansion | 0.547(21) | [16] | 96 |
| Field theory $D = 3$ | 0.541(14) | [18] | 87 |
| Field theory $D = 3$ | 0.536(19) | [16] | 96 |
| HT, LT series | 0.523(9) | [1] | 89 |
| MC, (a) | 0.550(12) | this work | 97 |
| MC, (b) | 0.567(16) | this work | 97 |
| MC, (c) | 0.560(10) | this work | 97 |

**Table 8.** In the second column we give results of [19] for the second moment correlation length $\xi_{2nd}$. In the third column we give our estimate for the singular part of the free energy density $f_s$, while the fourth column gives the resulting estimate for the universal combination $f_s\xi_{2nd}^3$.

| $\beta$ | $\xi_{2nd}$ | $f_s$ | $f_s\xi_{2nd}^3$ |
|---|---|---|---|
| 0.219 31 | 8.760(5) | 0.000 0524(22) | 0.0352(15) |
| 0.220 20 | 11.877(7) | 0.000 0212(9) | 0.0355(15) |
| | | | |
| 0.223 11 | 6.093(9) | 0.000 0377(9) | 0.0085(2) |
| 0.224 0 | 4.509(6) | 0.000 0927(22) | 0.0085(2) |

simulated. The results are given in table 8.

In both phases we have results for only two $\beta$-values. Since the results of these two $\beta$-values agree well we regard the results $f_s\xi^3 = 0.0355(15)$ and $f_s\xi^3 = 0.0085(2)$ for the high- and low-temperature phase as reliable estimates for the critical limits.

Note that the result depends on the normalization chosen here, in particular we have chosen to take the free energy per link rather than per site.

## 5. Conclusion

By careful scaling and finite-size scaling analysis of energy and specific heat data we obtained estimates for various critical quantities. Taking into account the simplicity of the approach, the results for the exponents $\nu$ and $\alpha$ are remarkably precise.

## References

[1] Liu A J and Fisher M E 1989 *J. Phys. A: Math. Gen.* **156** 35
[2] Privman V, Hohenberg P C and Aharony A 1991 *Phase Transitions and Critical Phenomena* vol 14, ed C Domb and J L Lebowitz (London: Academic)
[3] Talapov A L and Blöte H W J 1996 *Preprint* cond-mat/9603013
Talapov A L and Blöte H W J 1996 *J. Phys. A: Math. Gen.* **29** 5727
[4] Privman V 1990 *Finite Size Scaling and Numerical Simulation of Statistical Systems* ed V Privmann (Singapore: World Scientific)
[5] Cardy J 1996 *Scaling and Renormalization in Statistical Physics* (Cambridge: Cambridge University Press)

[6] Zinn-Justin J and Le Guillou J-C 1980 *Phys. Rev.* B **21** 3976
[7] Blöte H W J, Luijten E and Heringa J R 1995 *Preprint* cond-mat/9509016
Blöte H W J, Luijten E and Heringa J R 1995 *J. Phys. A: Math. Gen.* **28** 6289
[8] Kolesik M and Suzuki M 1995 *Physica* **215A** 138
[9] Nickel B G 1991 *Physica* **177A** 189
[10] Henkel M 1984 *J. Phys. A: Math. Gen.* **17** L795
Henkel M 1987 *J. Phys. A: Math. Gen.* **20** 3969
[11] Guttmann A J and Enting I G 1994 *J. Phys. A: Math. Gen.* **27** 8007
[12] Nickel B G and Rehr J J 1990 *J. Stat. Phys.* **61** 1
[13] Bhanot G, Creutz M, Glaessner U and Schilling K 1993 *Preprint* hep-lat/9312048
Bhanot G, Creutz M, Glaessner U and Schilling K 1994 *Phys. Rev.* B **49** 12 909
[14] Wolff U 1989 *Phys. Rev. Lett.* **62** 361
[15] Hasenbusch M and Pinn K 1997 *Preprint* cond-mat/9704075
Hasenbusch M and Pinn K 1997 *Physica* **245A** 366
[16] Guida R and Zinn-Justin J 1996 *Preprint* hep-th/9610223
Guida R and Zinn-Justin J 1997 *Nucl. Phys.* B **489** 626
[17] Nicoll J F and Albright P C 1985 *Phys. Rev.* B **31** 4576
Bervillier C 1986 *Phys. Rev.* B **31** 8141
[18] Bagnuls C, Bervillier C, Meiron D I and Nickel B G 1987 *Phys. Rev.* B **35** 3585
[19] Caselle M and Hasenbusch M 1997 *Preprint* hep-lat/9701007
Caselle M and Hasenbusch M 1997 *J. Phys. A: Math. Gen.* **30** 4963