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Ising universality in three dimensions: a Monte Carlo study

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Abstract. We investigate three Ising models on the simple cubic lattice by means of Monte Carlo methods and finite-size scaling. These models are the spin-$\frac{1}{2}$ Ising model with nearest-neighbour interactions, a spin-$\frac{1}{2}$ model with nearest-neighbour and third-neighbour interactions, and a spin-1 model with nearest-neighbour interactions. The results are in accurate agreement with the hypothesis of universality. Analysis of the finite-size scaling behaviour reveals corrections beyond those caused by the leading irrelevant scaling field. We find that the correction-to-scaling amplitudes are strongly dependent on the introduction of further-neighbour interactions or a third spin state. In a spin-1 Ising model, these corrections appear to be very small. This is very helpful for the determination of the universal constants of the Ising model. The renormalization exponents of the Ising model are determined as $y_t = 1.587$ (2), $y_h = 2.4815$ (15) and $y_i = -0.82$ (6). The universal ratio $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$ is equal to 0.6233 (4) for periodic systems with cubic symmetry. The critical point of the nearest-neighbour spin-$\frac{1}{2}$ model is $K_c = 0.2216546$ (10).

1. Introduction

According to insights such as the universality hypothesis, the nature of a phase transition does not depend on the microscopic details of a system but only on global properties such as dimensionality and symmetry of the order parameter. Thus, it is believed that most three-dimensional systems with short-range interactions and a scalar order parameter (such as density or unidirectional magnetization) belong to the Ising universality class. This implies that the critical exponents, as well as other universal quantities, are identical for all these models. This universality class comprises, in addition to anisotropic magnetic systems, also models for alloys, gas–liquid systems and liquid mixtures.

In the case of two-dimensional Ising-like models, the evidence that universality holds is very strong. However, in three dimensions, where exact results are scarce and numerical techniques tend to be less accurate than in two dimensions, the situation is less satisfactory. Numerical uncertainties in the renormalization exponents amount to the order of several times 10^{-3}. For many years the most accurate results have been those obtained by ε-, coupling-constant and series expansions [1–10], whereas recently quite accurate estimates have also been obtained by the coherent-anomaly method [11]. However, new possibilities of investigating Ising-like models are now arising in parallel with the availability of fast and relatively cheap computers. While many systems in the supposed Ising class may be simulated with the help of these, spin models offer a clear advantage, at least as far as a study of the universal properties is concerned. This is because of the ease and efficiency

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of the Monte Carlo method, in particular of cluster algorithms. Thus, results from Monte Carlo-based methods [12–21] tend to become increasingly accurate.

However, slight differences occur between recent results for the scaling dimensions. One possible explanation is that universality is not satisfied. In order to solve the issue of whether these deviations are real, it is desirable to obtain more accurate Monte Carlo data for the supposed universal quantities.

One problem that poses an obstacle to higher accuracies of these analyses is the presence of corrections to scaling. The dominant correction is attributed to an irrelevant renormalization exponent with an approximate value $y_i \simeq -0.83$ [8]. This means that the corrections decay relatively slowly and thus jeopardize the accuracy of the analysis. For this reason, we explore which modifications of the simple cubic Ising model with nearest-neighbour interactions can influence the amplitude of these corrections to scaling. If we can, in this way, suppress the irrelevant field, we may expect a decrease in the ill effects due to the corrections to scaling. One can, for instance, choose a different lattice structure. Series expansions using the body-centred cubic lattice [8] indicate that corrections to scaling are relatively small. However, here we prefer to introduce continuously variable parameters to adjust the irrelevant scaling field.

It is known [22] that the introduction of positive couplings with a range beyond the nearest neighbours in the simple cubic Ising model leads to a decrease of the correction-to-scaling amplitudes. We quote some preliminary results for the Hamiltonian

$$\mathcal{H}/k_B T = -K_{nn} \sum_{(nn)} s_i s_j - K_{2n} \sum_{(2n)} s_i s_j - K_{3n} \sum_{[3n]} s_i s_j - K_{\square} \sum_{\square} s_i s_j s_k s_l \qquad (1)$$

where (nn) indicates a sum over nearest-neighbour pairs, (2n) over second-neighbour pairs (diagonals of the elementary faces), [3n] over third-neighbour pairs (body diagonals in the elementary cubes) and $\square$ over four-spin products in all elementary faces of the cubic lattice. The associated couplings are denoted K_{nn}, K_{2n}, K_{3n} and $K_{\square}$, respectively. The spins s_i can assume the values $+1$ and -1. These results were obtained by Monte Carlo simulation on the Delft Ising System Processor [23, 24]; they indicated that the introduction of positive K_{2n}, K_{3n} or $K_{\square}$ reduces the correction-to-scaling amplitude. Third-neighbour couplings K_{3n} appear to be quite effective; for a ratio $K_{3n}/K_{nn} \approx 0.4$ the corrections become small. Much stronger second-neighbour couplings are required to obtain a similar effect [22].

Another approach is to introduce a third spin state $s_i = 0$: the spin-1 Ising model. The weight of the $s_i = 0$ state can be varied by means of a term $D \sum_i s_i^2$ in the Hamiltonian. Preliminary calculations showed that the corrections become small for $D \approx 0.7$. In our actual simulations we have used $D = \ln 2$, for reasons that will be explained in section 2.

Thus, we have selected the following three Ising models: the spin-$\frac{1}{2}$ Ising model with $K_{3n}/K_{nn} = 0$ (the nearest-neighbour model), with $K_{3n}/K_{nn} = 0.4$, and the spin-1 model with $D = \ln 2$ and nearest-neighbour interactions. The algorithms used to simulate these models are described in section 2. In addition to corrections to scaling, another obstacle to higher accuracies is the requirement of sufficiently accurate random numbers, in order to avoid biased results. In section 3 we comment on the quality of our random-number generators and we mention consistency checks to which the algorithms were subjected. An analysis of the results for the dimensionless ratio $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$ is given in section 4, followed by an analysis of the magnetic and temperature renormalization exponents in section 5. The results for the three models satisfy universality: they are equal within the statistical inaccuracies. Assuming universality, Q, as well as the critical points of the three models, can be obtained with a better precision, as is demonstrated in section 6. Finally, a discussion of these results in relation to the existing literature and to fundamental questions

concerning universality is presented in section 7. As an appendix, we present experimental results for critical exponents of a number of phase transitions that have been supposed to belong to the 3D Ising universality class.

2. Models and algorithms

The present Monte Carlo analysis concerns three different Ising models. These can be represented in terms of a spin-1 Hamiltonian on the simple cubic lattice:

$$\mathcal{H}/k_B T = -K_{nn} \sum_{\langle ij \rangle} s_i s_j - K_{3n} \sum_{[kl]} s_k s_l + D \sum_m s_m^2 \tag{2}$$

where nn and $\langle ij \rangle$ refer to nearest neighbours, and 3n and $[kl]$ to third-nearest neighbours (along body diagonals of the elementary cubes). The spins can assume three discrete values $s_i = 0, \pm 1$. The three models are specified in table 1.

Table 1. The ratio K_{3n}/K_{nn} and the value for D (see equation (2)) for the three models.

Model	K_{3n}/K_{nn}	D	Description of model
1	0	$-\infty$	Spin-$\frac{1}{2}$ model with nn couplings
2	0.4	$-\infty$	Spin-$\frac{1}{2}$ model with nn and 3n couplings
3	0	$\ln 2$	*Spin-1 model with nn couplings*

For $D = -\infty$ the $s_i = 0$ states are excluded and thus models 1 and 2 can be simulated by the Swendsen–Wang (SW) [25], the largest-cluster (LC) [26] or the Wolff [27] method. In cluster algorithms, one has to 'activate' a bond between two spins s_i and s_j, coupled with strength K_{ij}, with a probability $p(K_{ij})\delta_{s_i s_j}$, where $p(K_{ij}) \equiv [1 - \exp(-2K_{ij})]$. The presence of different sorts of bonds in model 2 thus leads to different bond probabilities but poses no further problems. If the bond is active, sites i and j belong to the same cluster. The simplest way to simulate this is to draw a random number for each bond and check whether it is smaller than $p(K_{ij})\delta_{s_i s_j}$. Following this procedure, the speed of the algorithm decreases as the number of interacting neighbours increases. When the couplings are small, a more efficient procedure is possible. As a first step in the SW or LC cluster formation process one obtains, for each type of bond K_{ij}, a list of bonds that should be activated if they connect equal spins. To this purpose, one introduces bond variables $b_{ij} = 0$ or 1; the probability that $b_{ij} = 1$ is equal to $p(K_{ij})$. The distribution $P(k) \equiv p(1-p)^{k-1}$, where we write p as an abbreviation for $p(K_{ij})$, expresses the probability that $(k-1)$ subsequent bond variables equal zero, while the kth bond variable is one. Thus one random number r can be transformed into an integer k:

$$k = 1 + [\ln(r)/\ln(1-p)] \tag{3}$$

where the square brackets denote the integer part. After evaluation of k, the next $(k-1)$ entries in the list of bond variables are set to zero, and the kth variable is set to one. By repetition of these steps a complete list of bond variables (for all bonds with strength K_{ij} in the lattice) is obtained. Such lists are generated for each different type of bond. After completion of these lists, the cluster formation is trivial. This procedure was found to improve the speed of the simulation of model 2 considerably. One may still choose between the SW or LC method. The latter method was observed to lead to shorter relaxation times and is therefore more efficient. The same principle was applied to Wolff-type simulations

of model 2. Random numbers are, as above, transformed into integers k. During the cluster formation, $(k-1)$ bonds of the pertinent type are skipped and the spin connected to the kth bond is added to the Wolff cluster if it has the right sign. This leads to a considerably faster Wolff algorithm, in particular because random-number generation is relatively time consuming (see section 3).

In the spin-1 case, transitions between zero and non-zero spin values require special attention. It is not immediately obvious how cluster algorithms could produce these transitions. We follow two different methods for the simulation of the spin-1 model. The first one uses a hybrid algorithm in which Metropolis sweeps alternate with cluster steps. The cluster algorithm acts on the non-zero spins only. Since we do not come close to the tricritical point where the ordered Ising phases meet the spin-zero phase, the regions of zero spins remain limited in size and we do not expect serious critical slowing down due to the equilibration between zero and non-zero spin values.

The second method uses a mapping on a spin-$\frac{1}{2}$ model. We consider a Hamiltonian with two spins $t_i = \pm 1$ and $u_i = \pm 1$ on site i (for all i) of the simple cubic lattice:

$$\mathcal{H}_h/k_B T = -M_1 \sum_{\langle ij \rangle} (t_i + u_i)(t_j + u_j) - M_2 \sum_m t_m u_m. \tag{4}$$

Using the transformation $s_i = (t_i + u_i)/2$ and $v_i = (1 + t_i)(1 - u_i)/4$, the partition function of this model is, up to a constant factor,

$$Z_h = \sum_{\{s_k\}} \left(\prod_{\langle ij \rangle} \exp\left[4M_1 s_i s_j\right] \prod_m \sum_{v_m=0}^{1-|s_m|} \exp\left[2M_2 s_m^2\right] \right) \tag{5}$$

with $s_i = 0, \pm 1$. Summation over the allowed values of v_m yields a factor 2 if $s_m = 0$. Thus

$$Z_h = 2^N \sum_{\{s_k\}} \exp\left[4M_1 \sum_{\langle ij \rangle} s_i s_j + (2M_2 - \ln 2) \sum_m s_m^2 \right] \tag{6}$$

where N denotes the number of spins in the system. This is, apart from the prefactor 2^N, precisely the partition sum for equation (2) for $K_{nn} = 4M_1$, $K_{3n} = 0$ and $D = \ln 2 - 2M_2$. Equation (4) may thus serve for the application of cluster algorithms to the spin-1 Ising model. The special choice $D = \ln 2$ leads to $M_2 = 0$ so that the spin-$\frac{1}{2}$ Hamiltonian simplifies. We have used three different methods to simulate the spin-1 model: the Metropolis-cluster (MLC) method, the full-cluster (FC) method and the Metropolis–Wolff (MW) method. The MLC method alternates one Metropolis sweep with one largest-cluster inversion, the MW method alternates one Metropolis sweep with 5 or 10 (this choice depends on the system size) Wolff steps. The FC method applies largest-cluster flips to the spin-$\frac{1}{2}$ representation of the model: no Metropolis sweeps are included here.

3. Random numbers and consistency tests

Significant systematic errors may be introduced in Monte Carlo simulations by using inadequate random-number generators. It is well known that linear congruential methods based on the truncation of 32-bit integers are unsuitable for long simulations. Even their period of about 10^9 would be too restrictive. On the other hand, also random-number generators based on binary feedback shift registers may introduce serious errors (see, e.g., [23, 28–31]). In most cases, the production rule selects two bits from the register and assigns their modulo-2 sum to the new bit. Thus the deviations from randomness are dominated by three-bit correlations. A number of algorithms of this type, using 127-bit shift registers

with a period in the order of 10^{38}, have been rejected on the basis of long tests [24] using Metropolis simulations of the critical Ising model. Recent tests by Ferrenberg *et al* [32] have shown that such deviations also occur when cluster algorithms are used together with random generators based on a generalized feedback shift register [33].

These findings apply to the Ising model on the square lattice, and use a comparison between simulations and exact results for finite systems. In the case of the three-dimensional Ising model, we have the practical difficulty that no exact results are available for general system sizes. One remaining possibility is a comparison between simulations with different realizations of the random-number generator and/or the spin-updating algorithm. Another possibility to check for systematic deviations is offered by numerical exact results for small systems. However, this test is not sufficient. It has been observed [34] that, in two dimensions, effects due to a random-number generator based on a generalized feedback shift register depend strongly on the system size and may be unobservable in small systems.

Systematic effects in 3D Ising model simulations are apparent from a comparison between finite-size results for the Binder cumulant [35] reported in [36] and [20], using the SW and LC methods. The random generator used in [36] was based on a generalized feedback shift register with length 502 [37], and that used in [20] combined such a generator of length 9689 with a multiplicative rule, by means of bitwise modulo-2 addition. The observed discrepancies may be attributed to the shift-register-based generator with length 502 [37], and become even more prominent in simulations of the Wolff type [37].

It is clear that, for the long simulations implied by the present analysis of the 3D Ising model, the random-number generators should be selected with great care. A systematic study of biases introduced by shift registers is necessary, in particular the dependence on the system size, shift-register length and the number of correlated bits. From simulations in two dimensions it appeared [38] that the deviations are scalable and become small for large system sizes and register lengths. Thus one may try to suppress systematic effects by using very long feedback shift registers [39]. But here we have chosen for a different method. This choice is based on the observation that the biases decrease when the number of bits in the production rule is increased [34, 38]. The bitwise modulo-2 addition of two sequences generated by three-bit production rules usually leads to a sequence in which the dominant correlation is one between 9 bits. Thus, we expected that, using a random generator of this type with sufficiently long registers, the systematic effects would be well below the statistical accuracy, in three dimensions as well as in two. The largest part of the present simulations in three dimensions used the production rules $a_i = a_{i-9218} \oplus a_{i-9689}$ and $b_i = b_{i-97} \oplus b_{i-127}$. These were combined by $r_i = a_i \oplus b_i$, where a_i, b_i and r_i are 32-bit integers, and $\oplus$ stands for bitwise modulo-2 addition. Most of the simulations of the nearest-neighbour model reported in [20] were performed using a random generator which combines a multiplicative sequence with a_i. No systematic differences between both types of results were observed, nor were there obvious differences between simulations of the SW, LC and Wolff types. Also in the case of models 2 and 3 we checked for the presence of significant differences between the result of the different types of spin-updating algorithms (see table 3) but none were found. This is consistent with the supposed high quality of the sequence r_i.

Therefore, we assume that the sequence r_i is sufficiently uncorrelated, so that the simulation results may serve as a standard to which data produced by means of other random generators can be compared. Thus, deviations in Wolff simulations of model 1, using 3-bit production rules, were determined and their scaling properties were analysed [40]. The results are qualitatively the same as in two dimensions, and are completely consistent with the picture that the deviations decrease rapidly with increasing system size

and shift-register length. No biases due to correlations of 5 or more bits were observed in Wolff simulations of the 3D Ising model.

As a further test, we have carried out exact numerical calculations of the dimensionless ratio $Q_L(K_{nn})$, the susceptibility χ, the energy-like quantity S_{nn} and the specific-heat-like quantity c_{nn}. For more precise definitions we refer to the next sections. These calculations apply to small systems with periodic boundaries: model 1 with sizes 3^3 and 4^3, and model 2 with size 3^3.

The calculations for the 3^3 systems involve a summation over 2^{27} distinct states. In view of the efficiency of the calculation, we divided these states into subsets such that the states in each subset are related by symmetries: spin and spatial inversions, translations and rotations. The number of subsets is 55 809, most of which contain 2592 states; this is the number of elements of the symmetry group of the 3^3 Ising lattice. Once a list of 'independent' states, one per subset, has been made, the calculation becomes rather simple. However, the 4^3 system is already too time-consuming unless treated carefully. The energy and the specific heat follow simply from the expansion coefficients given by Pearson [41]. For the magnetic quantities Q and χ we have used a perturbation expansion similar to that described by Saleur and Derrida [42]. Details are given in [20]. The results are summarized in table 2. The agreement between the Monte Carlo results and the exact numbers is quite satisfactory and does not suggest any problems with the random-number generator or other defects of the algorithm.

Table 2. Comparison between Monte Carlo and exact results for small system sizes. These data were taken at couplings $K_{nn} = 0.221\,653$ and $K_{nn} = 0.128\,006$ for models 1 and 2 respectively.

L	Model	Quantity	MC	Exact
3	1	Q	0.668 409 (20)	0.668 427
3	1	m^2	0.422 978 (19)	0.422 992
3	1	S_{nn}	1.434 382 (51)	1.434 418
3	1	c_{nn}	0.785 443 (53)	0.785 413
4	1	Q	0.659 755 (24)	0.659 779
4	1	m^2	0.331 228 (16)	0.331 204
4	1	S_{nn}	1.293 247 (40)	1.293 223
4	1	c_{nn}	0.977 559 (75)	0.977 575
3	2	Q	0.642 427 (20)	0.642 415
3	2	m^2	0.367 413 (17)	0.367 390
3	2	S_{nn}	1.134 852 (51)	1.134 791
3	2	c_{nn}	0.287 800 (19)	0.287 772

4. Test of universality

We have performed extensive simulations of models 1, 2 and 3, using the cluster methods described in section 2. The total simulation time amounts to approximately two years on three workstations. We chose systems with size $L \times L \times L$ and periodic boundaries. The lengths of the runs for the various models and methods are given in table 3 for each system size.

We sampled and analysed the dimensionless ratio:

$$Q_L(K_{nn}) = \frac{\langle m^2 \rangle_L^2}{\langle m^4 \rangle_L} \tag{7}$$

Table 3. Length of Monte Carlo runs in millions of sampled configurations. SW stands for Swendsen–Wang, LC for largest cluster and W for Wolff. For SW and LC, each new configuration corresponds with one cluster decomposition of the lattice. In the Wolff case, 5 (5W) or 10 (10W) Wolff clusters were flipped before a new configuration was used for data taking. For the spin-1 model (model 3) LC, 5W and 10W are preceded by M in order to indicate a Metropolis sweep through the lattice. FC indicates the full-cluster algorithm for the spin-1 model; it flips the largest cluster of a spin-$\frac{1}{2}$ version of the model.

Model	1				2				3			
L	SW	LC	5W	10W	SW	LC	5W	10W	FC	MLC	M5W	M10W
3	48	52	200			100	200		100	100	300	
4	160	40	200			150	100		100	100	300	
5	48	52	200			150	100		100	100	400	
6	48	52	200			150	100		100	100	400	
7	48	52	200			150	100		100	100	400	
8	48	52	200		10	140	100		100	100	400	
9	48	52	200		10	140	100		100	100	300	
10	48	52	200		10	140	100		100	100	300	
11	48	52	200			150	100		100	100	300	
12	28	72	200			150	100		100	100	200	
13	28	72	200			100	100				250	
14	28	72	200			100	100				200	
15	20	30		200		50		100			200	
16	20	30		150		50		100			200	
18	12	38		150		50		50			120	
20	20	10		70		50		50			120	
22	18	12		70		20		80			120	
24	8	12		80		20		80			150	
28	10	10		100		20		80			50	50
32	2	18		180		25		75				100
40		10		90		20		80				100

where L is the finite size of the model and m the magnetization density. We use the renormalization language in order to derive the expected finite-size scaling behaviour of Q_L. By $f(t, h, u, L^{-1})$ we denote the free-energy density as a function of the temperature and magnetic scaling fields, an irrelevant field and the finite-size field [43, 44]. Here, we define the free energy as $F = \ln Z$, so without the normal factor $-1/k_B T$. Its behaviour under renormalization with a scale factor l is

$$f(t, h, u, L^{-1}) = l^{-d} f(l^{y_t} t, l^{y_h} h, l^{y_i} u, l/L) + g(t, h) \tag{8}$$

where y_t, y_h and y_i are the pertinent renormalization exponents, $d = 3$ is the dimensionality and g is the analytic part of the transformation. By differentiating k times with respect to h, and choosing $l = L$ and $h = 0$, one obtains

$$f^{(k)}(t, u, L^{-1}) = L^{k y_h - d} f^{(k)}(L^{y_t} t, L^{y_i} u, 1) + g^{(k)}(t) \tag{9}$$

where the dependence on h is no longer needed and therefore suppressed. The expectation values of the second and fourth magnetization moments require differentiations of the free energy with respect to the physical magnetic field H:

$$\langle m^2 \rangle = L^{-d} \left(\frac{\partial^2 f}{\partial H^2} \right)_{H=0} \tag{10}$$

Table 4. Numerical results for the dimensionless ratio $Q_L = \langle m^2 \rangle_L^2 / \langle m^4 \rangle_L$ for the three Ising models defined in section 2. These data were taken at couplings $K_{nn} = 0.221\,653$, $0.128\,006$ and $0.393\,410$ for models 1, 2 and 3, respectively.

L	Model 1	Model 2	Model 3
3	0.668 39 (2)	0.642 44 (3)	0.618 94 (2)
4	0.659 76 (2)	0.631 64 (3)	0.621 34 (2)
5	0.653 73 (2)	0.626 42 (3)	0.622 42 (2)
6	0.649 19 (2)	0.623 70 (3)	0.622 73 (2)
7	0.645 79 (3)	0.622 17 (3)	0.622 77 (2)
8	0.643 18 (3)	0.621 26 (3)	0.622 88 (2)
9	0.641 07 (3)	0.620 87 (3)	0.622 80 (3)
10	0.639 43 (3)	0.620 51 (4)	0.622 80 (3)
11	0.638 03 (3)	0.620 45 (4)	0.622 75 (3)
12	0.636 88 (3)	0.620 26 (4)	0.622 72 (3)
13	0.635 91 (4)	0.620 30 (4)	0.622 67 (5)
14	0.635 14 (4)	0.620 34 (5)	0.622 62 (5)
15	0.634 41 (3)	0.620 41 (4)	0.622 66 (5)
16	0.633 76 (4)	0.620 50 (5)	0.622 47 (5)
18	0.632 70 (4)	0.620 57 (6)	0.622 48 (7)
20	0.631 87 (6)	0.620 81 (6)	0.622 30 (8)
22	0.631 17 (6)	0.621 01 (6)	0.622 11 (8)
24	0.630 52 (6)	0.620 98 (7)	0.622 01 (7)
28	0.629 58 (6)	0.621 42 (7)	0.621 77 (9)
32	0.628 79 (5)	0.621 74 (8)	0.621 29 (8)
40	0.627 61 (8)	0.622 50 (9)	0.620 50 (9)

and

$$\langle m^4 \rangle = L^{-3d} \left(\frac{\partial^4 f}{\partial H^4} \right)_{H=0} + 3L^{-2d} \left(\frac{\partial^2 f}{\partial H^2} \right)_{H=0}^2 . \tag{11}$$

The Ising up–down symmetry implies that h is an odd function of H. Thus the correspondence between the derivatives with respect to h and H is

$$\frac{\partial^2 f}{\partial H^2} = f^{(2)} \left(\frac{\partial h}{\partial H} \right)^2 \tag{12}$$

and

$$\frac{\partial^4 f}{\partial H^4} = f^{(4)} \left(\frac{\partial h}{\partial H} \right)^4 + 4 f^{(2)} \frac{\partial h}{\partial H} \frac{\partial^3 h}{\partial H^3} \tag{13}$$

where, as before, $f^{(k)}$ stands for $\partial^k f / \partial h^k$ and all derivatives with respect to H are evaluated at $H = 0$. In the vicinity of the finite-size limit (t small and L finite), we may Taylor-expand the right-hand side of equation (9) in t and u. After the appropriate substitutions, the finite-size expansion of $Q_L(K_{nn})$ follows as

$$\begin{aligned} Q_L(K_{nn}) = Q &+ a_1(K_{nn} - K_c) L^{y_t} + a_2(K_{nn} - K_c)^2 L^{2y_t} + a_3(K_{nn} - K_c)^3 L^{3y_t} + \cdots \\ &+ b_1 L^{y_1} + b_2 L^{y_2} + \cdots \end{aligned} \tag{14}$$

where the a_i and b_i are non-universal coefficients and $y_2 = d - 2y_h$. The last term is due to the field dependence of the analytic part g in equation (9). The nonlinear dependence of h on H leads to even more rapidly decaying contributions (not shown). Terms of the same form, but with different exponents, may be due to other irrelevant fields. Because powers

Table 5. Results of a data analysis of the three models, including system sizes $L \geqslant 7$ for model 1 and $L \geqslant 6$ for models 2 and 3. Besides the ratio Q, the critical couplings K_c and the non-universal coefficients a_1, a_2, b_1 and b_2 are listed.

	Model 1	Model 2	Model 3
Q	0.6232 (8)	0.6229 (3)	0.6231 (2)
K_c	0.221 6542 (8)	0.128 0034 (4)	0.393 4214 (8)
a_1	0.862 (10)	1.43 (4)	0.659 (6)
a_2	0.54 (6)	1.5 (2)	0.352 (15)
b_1	0.102 (10)	−0.043 (4)	0.001 (2)
b_2	0.11 (3)	0.351 (13)	−0.018 (9)

Table 6. Results of a data analysis of the three models, where all system sizes $L \geqslant 5$ were used and a third correction term was included. Besides the ratio Q, the non-universal coefficients a_1, a_2, b_1, b_2 and b_3 and the critical couplings K_c are listed.

	Model 1	Model 2	Model 3
Q	0.6235 (7)	0.6231 (4)	0.6235 (3)
K_c	0.221 6547 (8)	0.128 0036 (5)	0.393 4224 (10)
a_1	0.862 (9)	1.43 (4)	0.659 (6)
a_2	0.54 (6)	1.5 (2)	0.352 (15)
b_1	0.098 (9)	−0.045 (6)	−0.004 (3)
b_2	0.15 (4)	0.37 (2)	0.02 (2)
b_3	−4.9 (8)	−1.4 (8)	−2.0 (7)

of the geometric factor $\partial h/\partial H$ cancel in the first term, Q is a universal constant (related to the Binder cumulant [35]).

The bulk of the numerical data were taken at couplings $K_{nn} = 0.221\,653$, 0.128 006 and 0.393 410 for models 1, 2 and 3 respectively, close to the critical points. The results in terms of Q_L are shown in table 4. A few points at somewhat different couplings were included in order to estimate the coefficients a_i in equation (14). The procedure of the analysis is as follows. We computed $Q_L(K_{nn})$ for several values of L, K_{nn} (near the critical points K_c) for the three models and fitted equation (14) to the data. The following parameters were used as input: $y_t = 1.584$ (4) (from ε-expansion [6]; because the data were taken at couplings so close to the critical points, the results of the fits are practically independent of the precise value); $y_i = -0.83$ (5) (from series expansions [8]; the fit is rather sensitive to the precise value) and $y_2 = -1.963$ (3) (from renormalization arguments given above and the ε-expansion result [6] for the magnetic exponent; the fit is insensitive to the precise value). The results are summarized in table 5. It is stressed that the error margins quoted here include the uncertainty due to the possible variations in y_i, y_t and y_2 (y_h). The fits for model 1 indicated that system sizes $L < 7$ should be discarded; they reveal finite-size effects not included in equation (14), exceeding the statistical error margins. The fits for models 2 and 3, which exhibit much smaller finite-size effects, include system sizes $L \geqslant 6$. The fit for model 2 clearly reveals a correction with exponent $y_2 \approx -1.96$. In fact, the large residuals in the absence of such a correction demonstrated its presence. As indicated above, this correction may arise from the analytic part of the transformation, although we cannot exclude contributions due to a second irrelevant exponent. Since there is no obvious reason why this term should be absent in general, we have included it in the fitting procedures for models 1 and 3 as well. Furthermore, we observe that the amplitude b_1 of the leading

correction to scaling can be suppressed. This amplitude has become quite small in the spin-1 model (model 3) and has even changed sign in model 2. In model 1, the amplitude b_1 is relatively large and we have attempted to determine the irrelevant exponent by including it as a parameter in the fit. However, for an acceptable fit it was necessary to include the correction term $b_2 L^{y_2}$. Unfortunately, this frustrated the determination of y_i for model 1: if we fixed $y_2 = -1.963$ the exponent y_i shifted towards y_2 and if we included both y_i and y_2 as free parameters, they approached the same value.

In order to take into account the finite-size effects revealed by the system sizes omitted in the previous fits, we have repeated our data analysis with an additional correction to scaling $b_3 L^{y_3}$ in equation (14), where $y_3 = -2y_h$. This term, which is due to the nonlinear dependence of the magnetic scaling field on the physical magnetic field, enabled us to include all system sizes $L \geqslant 5$ for models 1, 2 and 3 in the analysis. The results, which are presented in table 6, are consistent with those obtained previously. Again, the error margins quoted include the uncertainty due to the errors in y_i, y_t and y_h. These data satisfy universality within a margin of less than 10^{-3}. To our knowledge, this is the most precise verification so far for 3D Ising-like models.

5. Determination of the critical dimensions

This section presents finite-size analyses of the energy, specific heat, spin–spin correlations over half the system size, susceptibility, the temperature derivative of the susceptibility and the temperature derivative of the ratio Q_L. Taking $h = 0$ and $l = L$ in equation (8) leads to

$$f(t, u, L^{-1}) = L^{-d} f(L^{y_t} t, L^{y_t} u, 1) + g(t). \tag{15}$$

Expansion in t and u yields

$$\begin{aligned} f(t, u, L^{-1}) = L^{-d}(f^{(0,0)} + f^{(1,0)} L^{y_t} t + \tfrac{1}{2} f^{(2,0)} L^{2y_t} t^2 + \cdots \\ + f^{(0,1)} L^{y_t} u + f^{(1,1)} L^{y_t + y_t} tu + \cdots) + g^{(0)} + g^{(1)} t + \tfrac{1}{2} g^{(2)} t^2 + \cdots \end{aligned} \tag{16}$$

where $f^{(k,l)}$ stands for $\partial^{k+l} f / \partial^k t \partial^l u$. The finite-size scaling behaviour of the energy and that of the specific heat follow by differentiation.

5.1. The energy

During the simulations, the nearest-neighbour sum $S_{nn} = \sum_{\langle nn \rangle} s_i s_j$ was sampled. For model 1, this sum is proportional to the energy; for models 2 and 3 its scaling behaviour is similar. Its expectation value is equal to

$$\langle S_{nn} \rangle = \frac{\partial f}{\partial K_{nn}} = \frac{\partial f}{\partial t} \frac{\partial t}{\partial K_{nn}} + \frac{\partial f}{\partial u} \frac{\partial u}{\partial K_{nn}}. \tag{17}$$

The finite-size scaling behaviour of this quantity thus follows by differentiating equation (16) and substitution in equation (17):

$$\begin{aligned} \langle S_{nn} \rangle = c_0 + c_1 (K_{nn} - K_c) + \cdots + L^{y_t - d}[a_0 + a_1 (K_{nn} - K_c) L^{y_t} + a_2 (K_{nn} - K_c)^2 L^{2y_t} \\ + \cdots + b_1 L^{y_i} + b_2 L^{y_i - y_t} + \cdots] \end{aligned} \tag{18}$$

where the a_i, b_i and c_i are unknown coefficients. Analysis of the numerical results for $\langle S_{nn} \rangle$ enables a determination of these coefficients and of y_t. The dominant singular term in equation (18) is the one with amplitude a_0. The $(K_{nn} - K_c)$-dependent term with amplitude c_1 is dominated by the term with coefficient a_1 and has therefore been omitted from the scaling formula. Since the bulk of the data were taken very close to the critical points, only

linear and quadratic terms in $(K_{nn} - K_c)$ were included. Without the correction term with coefficient b_2, we had to exclude system sizes $L < 8$ in the analysis of model 1, in order to obtain an acceptable residual. The resulting estimate for y_t is: 1.586 (6). Inclusion of the second irrelevant term enabled us to include all system sizes $L \geqslant 5$. For consistency, we have included this term in the data analyses for models 2 and 3 as well. Table 7 summarizes the results obtained from fits according to equation (18), at the critical points listed in table 6, for system sizes $L \geqslant 5$. Since the singular behaviour of $\langle S_{nn} \rangle$ is rather weak, the results $y_t \approx 1.59$ for each of the three models are relatively inaccurate but consistent with the existing literature. The uncertainty due to the errors in K_c and y_i has been included in the error margins.

Table 7. Results of a data analysis of the nearest-neighbour sum $\langle S_{nn} \rangle$ for the three models.

	Model 1	Model 2	Model 3
y_t	1.599 (8)	1.589 (9)	1.591 (7)
c_0	0.99051 (8)	0.66298 (9)	0.59451 (6)
a_0	2.14 (6)	2.20 (7)	1.73 (4)
b_1	0.14 (15)	0.16 (17)	0.04 (12)
b_2	−2.0 (4)	−0.6 (4)	−0.9 (3)

5.2. *The specific heat*

The fluctuations in S_{nn} are related to the specific-heat-like quantity

$$c_{nn} = K_{nn}^2 \frac{\partial^2 f}{\partial K_{nn}^2} = K_{nn}^2 [\langle S_{nn}^2 \rangle - \langle S_{nn} \rangle^2]. \tag{19}$$

We consider f as a function of the scaling fields t and u:

$$c_{nn} = K_{nn}^2 \left[\frac{\partial f}{\partial t} \frac{\partial^2 t}{\partial K_{nn}^2} + \frac{\partial f}{\partial u} \frac{\partial^2 u}{\partial K_{nn}^2} + \frac{\partial^2 f}{\partial t^2} \left(\frac{\partial t}{\partial K_{nn}} \right)^2 + 2 \frac{\partial^2 f}{\partial t \partial u} \frac{\partial t}{\partial K_{nn}} \frac{\partial u}{\partial K_{nn}} + \frac{\partial^2 f}{\partial u^2} \left(\frac{\partial u}{\partial K_{nn}} \right)^2 \right]. \tag{20}$$

Taking the appropriate derivatives in equation (16) and collecting the leading analytic and singular terms leads to

$$c_{nn} = p_0 + p_1 (K_{nn} - K_c) + \cdots + L^{2y_t - d} [q_0 + q_1 (K_{nn} - K_c) L^{y_t} + q_2 (K_{nn} - K_c)^2 L^{2y_t} + \cdots + r_1 L^{y_i} + \cdots] + L^{y_t - d} [s_0 + s_1 (K_{nn} - K_c) L^{y_t} + \cdots]. \tag{21}$$

The numerical results for c_{nn} of models 1–3 were subjected to a fit of this form with $y_i = -0.83$ and the K_c values in table 6 as input parameters. The terms with amplitudes p_1 and s_1 are dominated by that with amplitude q_1 and were omitted from the fit formula, as well as quadratic terms in $(K_{nn} - K_c)$. System sizes $L < 6$ display finite-size corrections not included in equation (21) and were discarded. The main results of these fits are shown in table 8, where the error margins include the uncertainties in K_c and y_i. Also in the present case we find consistent, but inaccurate values of y_t. This may be related to the fact that the leading power of L in equation (21) is close to zero, so that this term, which has the coefficient q_0, interferes with the term with coefficient p_0.

Table 8. Results of a data analysis of the specific-heat-like quantity c_{nn} obtained from the fluctuations of the nearest-neighbour sum S_{nn} for each of the three models.

	Model 1	Model 2	Model 3
y_t	1.60 (2)	1.579 (15)	1.59 (2)
p_0	−0.8 (7)	−0.6 (3)	−3 (2)
q_0	1.5 (5)	0.8 (3)	3.5 (14)
q_1	2.2 (2)	1.39 (12)	3.7 (4)
r_1	−0.4 (4)	0.11 (14)	0.0 (9)
s_0	−0.4 (3)	−0.24 (13)	−1.0 (7)

5.3. The spin–spin correlation function

In our simulations, we have sampled the spin–spin correlation function $g(r)$,

$$g(r) = \langle s(\mathbf{0})s(r)\rangle \tag{22}$$

over half the system size ($r = L/2$), for even system sizes. This quantity can be derived from the free energy F by differentiating with respect to two physical magnetic fields H_0 and H_r, which couple to the spins at positions $\mathbf{0}$ and r, respectively. We consider the two fields as independent and find

$$g(r) = \left(\frac{\partial^2 F}{\partial H_0 \partial H_r}\right)_{H_0=H_r=0} = \left(\frac{\partial^2 F}{\partial h_0 \partial h_r}\frac{\partial h_0}{\partial H_0}\frac{\partial h_r}{\partial H_r}\right)_{H_0=H_r=0} \tag{23}$$

where h denotes the leading magnetic scaling field and the derivatives with respect to this field are evaluated at $h_0 = h_r = 0$. Using equation (9) one obtains upon expansion in t and u the scaling behaviour of the correlation function,

$$g = L^{2y_h-2d}[a_0 + a_1(K_{nn} - K_c)L^{y_t} + a_2(K_{nn} - K_c)^2 L^{2y_t} + \cdots + b_1 L^{y_i} + \cdots] \tag{24}$$

where the coefficients a_i and b_i are different from those in equation (18).

We have fitted the terms shown in (24) to our data. The large residuals for all three models strongly suggested the presence of an additional correction to scaling $b_2 L^{y'}$. A problem for the determination of y' is the presence of the leading correction term $b_1 L^{y_i}$. Only in the spin-1 model (model 3), where the amplitude b_1 is small and the term thus may be omitted, was a reasonable determination possible, yielding $y' = -2.1$ (1). This could be a second temperature-like irrelevant exponent, although we have not observed it in the analysis of the ratio Q or the energy-like quantity S_{nn}. In Q, it may have been masked by the term $b_2 L^{y_2}$, but this is less likely for S_{nn}, where the exponent of the second correction term is approximately equal to -2.4. On the other hand, the contribution $b_2 L^{y'}$ could, in principle, be due to a second relevant magnetic exponent $\tilde{y}_h$. Taking into account the dependence of F on an additional magnetic scaling field $\tilde{h}$ yields

$$g(r) = \frac{\partial^2 F}{\partial h_0 \partial h_r}\left(\frac{\partial h}{\partial H}\right)^2 + \left(\frac{\partial^2 F}{\partial h_0 \partial \tilde{h}_r} + \frac{\partial^2 F}{\partial \tilde{h}_0 \partial h_r}\right)\frac{\partial h}{\partial H}\frac{\partial \tilde{h}}{\partial H} + \frac{\partial^2 F}{\partial \tilde{h}_0 \partial \tilde{h}_r}\left(\frac{\partial \tilde{h}}{\partial H}\right)^2. \tag{25}$$

This results in extra terms proportional to $L^{y_h+\tilde{y}_h-2d}$ and $L^{2\tilde{y}_h-2d}$ in the scaling formula for g, corresponding to correction terms $L^{\tilde{y}_h-y_h}$ and $L^{2\tilde{y}_h-2y_h}$ in equation (24). Remarkably, the second magnetic exponent $\tilde{y}_h = 0.42$ [15, 19] has just the right value. However, its identification in terms of a redundant operator [15, 19] would exclude its contribution to thermodynamic quantities. Table 9 shows the main results of an analysis for system sizes $L \geqslant 8$, where we have included three correction terms, $b_1 L^{y_i}$, $b_2 L^{y'}$ and $b_3 L^{2y'}$, with the

exponents y_i and y' fixed at -0.83 and -2.1, respectively. We have not included the term proportional to L^{2y_i} because b_1 is already quite small. The errors quoted in the table include the uncertainties in K_c, y_t, y_i and y'. The estimates of y_h for each of the three models are consistent and in agreement with the existing literature.

Table 9. Results of a data analysis of the spin–spin correlation function g for the three models.

	Model 1	Model 2	Model 3
y_h	2.480 (2)	2.482 (3)	2.482 (3)
a_0	0.77 (2)	0.547 (15)	0.453 (14)
a_1	2.45 (4)	3.07 (6)	1.18 (2)
a_2	3.44 (14)	7.2 (3)	1.30 (3)
b_1	−0.22 (10)	0.08 (8)	0.01 (7)

Table 10. Results of a data analysis of the susceptibility χ for the three models.

	Model 1	Model 2	Model 3
y_h	2.4812 (11)	2.4817 (10)	2.4826 (9)
c_0	−0.6 (2)	−0.20 (7)	−0.50 (6)
a_0	1.559 (16)	1.126 (9)	0.926 (7)
a_1	4.88 (6)	6.16 (8)	2.36 (3)
a_2	6.9 (4)	14.4 (7)	2.62 (7)
b_1	−0.37 (5)	0.14 (3)	−0.05 (2)

5.4. The magnetic susceptibility

The magnetic susceptibility χ can be calculated from the average square magnetization, which is sampled in the Monte Carlo simulations,

$$\chi = L^d \langle m^2 \rangle. \tag{26}$$

Using equations (9), (10) and (12), we find for the finite-size scaling behaviour:

$$\chi = g^{(2)}(t) + L^{2y_h - d} f^{(2)}(L^{y_t} t, L^{y_i} u, 1) \tag{27}$$

which yields, upon expansion in t and u,

$$\chi = c_0 + c_1(K_{nn} - K_c) + \cdots + L^{2y_h - d}[a_0 + a_1(K_{nn} - K_c)L^{y_i} + a_2(K_{nn} - K_c)L^{2y_i} + b_1 L^{y_i} + \cdots] \tag{28}$$

where the a_i, b_i and c_i are non-universal coefficients. In table 10, we present the results of fits of the susceptibility for the models 1–3 at the critical points listed in table 6. For model 1, system sizes $L \geqslant 8$ were included in the analysis and for models 2 and 3, which exhibit smaller corrections to scaling, all system sizes $L \geqslant 6$ were used. The coefficient c_1 in equation (28) was set to zero in all analyses, because the term containing it is much smaller than the $(K_{nn} - K_c)$-dependent term with amplitude a_1. The errors include the margins due to the uncertainties in K_c, y_i and y_t. The ratio between the coefficients a_0 for the three models is in excellent agreement with the ratio between the coefficients a_0 in table 9. The same holds for the coefficients a_1, a_2 and b_1.

On the other hand, one might derive the scaling formula for χ from that of the spin–spin correlation function g, because χ is equal to the spatial integral of g,

$$\chi = \int g(r) r^{d-1} \mathrm{d}r. \tag{29}$$

Since the integral in equation (29) preserves the form of the corrections to scaling in g, we expect the same type of corrections in the correlation function and the susceptibility. Only the terms proportional to $c_0, c_1, \ldots$ in (28), which arise from the analytical part of the free energy, are absent in equation (24). These contributions come from the small-r cutoff in equation (29). Thus, we have included in the scaling formula the additional corrections that we observed in the analysis of the correlation function. As the term proportional to $L^{y'}$ interferes with the constant contribution c_0, we have only included the correction $b_2 L^{2y'}$. This allowed us to include system sizes $L \geqslant 5$ for all three models. The results, which are presented in table 11, are consistent with those obtained in the previous analysis. Now, the errors also include the margins due to the uncertainty in y'. Just as in the analysis of the correlation function, we find consistent results for y_h, which are in agreement with the literature. However, the values for y_h are more accurate than those obtained in the previous subsection and our resulting estimate for the magnetic renormalization exponent is $y_h = 2.4815$ (15). The error margin amounts to two standard deviations, in order to take into account any arbitrariness in the fit formula.

Table 11. Results of a data analysis of the susceptibility χ for the three models, where all system sizes $L \geqslant 5$ were employed and an additional correction to scaling was included in the scaling formula.

	Model 1	Model 2	Model 3
y_h	2.4813 (11)	2.4810 (14)	2.4817 (13)
c_0	−0.5 (2)	0.0 (2)	−0.33 (13)
a_0	1.558 (15)	1.134 (13)	0.934 (10)
a_1	4.87 (6)	6.18 (8)	2.37 (3)
a_2	6.9 (3)	14.5 (7)	2.64 (7)
b_1	−0.37 (5)	0.10 (6)	0.01 (13)
b_2	−5 (2)	−2.9 (16)	−2.6 (13)

5.5. *The temperature derivative of* χ

In the simulations, we have also sampled the correlation between m^2 and S_{nn}. This allows us to calculate the temperature derivative of the susceptibility,

$$\frac{\partial \chi}{\partial K_{nn}} = L^d(\langle m^2 S_{nn}\rangle - \langle m^2\rangle\langle S_{nn}\rangle). \tag{30}$$

The scaling behaviour of this quantity can be derived directly from that of the susceptibility, equation (28),

$$\frac{\partial \chi}{\partial K_{nn}} = c_1 + \cdots + L^{2y_h+y_t-d}[a_1 + 2a_2(K_{nn} - K_c)L^{y_t} + 3a_3(K_{nn} - K_c)^2 L^{2y_t} + \cdots + \tilde{b}_1 L^{y_t} + \cdots]. \tag{31}$$

The term with amplitude $\tilde{b}_1$ comes from a term proportional to $(K_{nn} - K_c)L^{y_h+y_t}$, included in the ellipsis in equation (28). Just as in the analysis of the spin–spin correlation function, the residuals for all three models indicated the presence of an additional correction to scaling

$\tilde{b}_2 L^{y'}$, which indeed follows from the discussion in the previous subsection. Table 12 shows the results of an analysis at the critical points listed in table 6, where this additional correction was included. All system sizes $L \geqslant 6$ were used. The exponents y_i and y' were kept fixed at -0.83 and -2.1, respectively. The error margins include the uncertainties in K_c, y_i and y'. The fit yields values for $(2y_h + y_t)$ and the results for y_t have been obtained by fixing y_h at the best estimate from the previous subsection. This implies an additional error margin of 0.003 for y_t. For models 1 and 3, there is a reasonable agreement between the amplitudes a_1 and a_2 as shown in table 11 and those in table 12. The differences are explained from the approximations in the scaling formulae. For model 2, no agreement is expected, because an additional term arises in the temperature derivative of the susceptibility due to the temperature dependence of K_{3n} (the ratio between K_{nn} and K_{3n} is fixed).

Table 12. Results of a data analysis of the temperature derivative of the susceptibility $\partial\chi/\partial K_{nn}$ for the three models, where all system sizes $L \geqslant 6$ were employed and an additional correction to scaling was included in the scaling formula.

	Model 1	Model 2	Model 3
y_t	1.585 (3)	1.584 (4)	1.587 (4)
c_1	31 (11)	1 (9)	12 (7)
a_1	5.11 (9)	3.73 (6)	2.39 (5)
a_2	6.46 (10)	8.04 (9)	2.53 (3)
a_3	−2.4 (4)	−4.4 (5)	−0.53 (5)
$\tilde{b}_1$	−2.6 (3)	0.1 (3)	−0.1 (2)
$\tilde{b}_2$	−13 (3)	−6 (2)	−5.5 (16)

5.6. The temperature derivative of Q

Another quantity of interest correlates the magnetization distribution with the nearest-neighbour sum S_{nn}:

$$\frac{\partial Q}{\partial K_{nn}} = Q\left(2\frac{\langle m^2 S_{nn}\rangle - \langle m^2\rangle\langle S_{nn}\rangle}{\langle m^2\rangle} - \frac{\langle m^4 S_{nn}\rangle - \langle m^4\rangle\langle S_{nn}\rangle}{\langle m^4\rangle}\right). \tag{32}$$

The determination of m and S_{nn} during the simulations enables the sampling of this quantity with very little additional effort. Returning to equation (14) and noting that the ellipses include terms proportional to $(K_{nn} - K_c)L^{y_i+y_i}$ and to $(K_{nn} - K_c)L^{y_2}$, we obtain the finite-size scaling behaviour

$$\frac{\partial Q}{\partial K_{nn}} = L^{y_i}[u_0 + u_1(K_{nn} - K_c)L^{y_i} + u_2(K_{nn} - K_c)^2 L^{2y_i} + \cdots + vL^{y_i} + wL^{y_2 - y_i} + \cdots]. \tag{33}$$

The numerical data for the three models were subjected to a fit on the basis of equation (33), where we have included system sizes $L \geqslant 7$ for model 1 and $L \geqslant 5$ for models 2 and 3. In this case the leading power of L stands well apart from the less singular terms and the results for y_t (table 13; uncertainties in K_c, y_i and y_h are included in all error margins) appear to be more accurate than those in the preceding subsections. The results suggest that the correction due to the leading irrelevant field is very small. Therefore we have repeated our analysis with v fixed to zero. We expect this to work especially well for models 2 and 3, where the irrelevant field is notably smaller than that in the first model. Indeed, we have obtained accurate and consistent results for the models 2 and 3, as shown

in table 14. These results, together with those presented in table 13, lead us to our final result, $y_t = 1.587\ (2)$. Just as in the final result for y_h in section 5.4, we quote here an error margin of two standard deviations.

Table 13. Results of a data analysis of the derivative of the quantity Q with respect to the nearest-neighbour coupling K_{nn}.

	Model 1	Model 2	Model 3
y_t	1.589 (2)	1.587 (2)	1.5878 (14)
u_0	1.341 (14)	1.351 (9)	1.057 (6)
u_1	−0.21 (3)	0.00 (5)	−0.012 (9)
u_2	−10.7 (6)	−28.3 (11)	−4.80 (12)
v	−0.01 (6)	0.00 (3)	0.02 (2)
w	−0.5 (2)	0.46 (8)	−0.13 (5)

Table 14. Results of a data analysis of the derivative of the quantity Q with respect to the nearest-neighbour coupling K_{nn} for models 2 and 3, where the leading correction to scaling has been omitted.

	Model 2	Model 3
y_t	1.5868 (3)	1.5867 (2)
u_0	1.3512 (11)	1.0623 (7)
u_1	0.00 (5)	−0.013 (9)
u_2	−28.3 (11)	−4.81 (12)
w	0.457 (15)	−0.091 (9)

Table 15. Results of a data analysis assuming universality of $Q_L = \langle m^2 \rangle_L^2 / \langle m^4 \rangle_L$ for the three investigated Ising models. System sizes $L \geqslant 8$ were included in the fit. The table lists non-universal parameters: the critical points and the amplitudes of the *two* correction terms. Furthermore, this analysis yielded the universal parameters $Q = 0.6232\ (2)$ and $y_i = -0.78\ (3)$.

	Model 1	Model 2	Model 3
K_c	0.221 6550 (6)	0.128 0037 (4)	0.393 4217 (8)
b_1	0.086 (8)	−0.040 (5)	−0.001 (2)
b_2	0.18 (3)	0.34 (2)	0.000 (14)

6. Simultaneous fits for the three models

Considering the results in the preceding sections, it is reasonable to assume now that universality is *exactly* satisfied for the three models under investigation. Thus we made a fit of the combined data for the ratio Q, allowing only single values of Q and y_i for the three models. The other parameters a_1, a_2, K_c, b_1 and b_2 (see equation (14)) are non-universal and occur in triplicate. Now, system sizes $L < 8$ had to be discarded, except when an additional correction to scaling proportional to L^{-2y_h} was added to the scaling formula. In the latter case, all system sizes $L \geqslant 5$ could be included. Some of the results

Table 16. Results of a data analysis assuming universality of $Q_L = \langle m^2 \rangle_L^2 / \langle m^4 \rangle_L$ for the three investigated Ising models. System sizes $L \geqslant 5$ were included in the fit. The table lists non-universal parameters: the critical points and the amplitudes of the *three* correction terms. Furthermore, this analysis yielded the universal parameters $Q = 0.6233$ (2) and $y_i = -0.82$ (3).

	Model 1	Model 2	Model 3
K_c	0.221 6546 (5)	0.128 0039 (4)	0.393 4220 (7)
b_1	0.096 (7)	−0.046 (5)	−0.002 (2)
b_2	0.15 (3)	0.38 (2)	0.007 (12)
b_3	−4.9 (8)	−1.7 (7)	−1.7 (5)

are summarized in tables 15 and 16, respectively, where the error margins include the uncertainty introduced by the error in y_t and y_h.

Let us now compare the results of the various fits. In the first place, we see that the results in tables 15 and 16 are consistent, just as was the case for tables 5 and 6 in section 4. Also the values for the universal quantity Q, 0.6232 (2) and 0.6233 (2), respectively, agree. Secondly, the simultaneous fit with only the first two corrections to scaling (table 15) yields results that are consistent with those presented in table 5. Only the amplitude b_2 and the critical coupling K_c for model 1 appear to be somewhat too low in table 5, as we already had seen from the second fit in section 4. Finally, when we compare the results in tables 6 and 16, i.e. including a third correction to scaling, as well as the corresponding Q values, we see a very good agreement. These comparisons, in addition to the fact that the term $b_3 L^{y_3}$ allowed us to include all system sizes $L \geqslant 5$, lead us to the conclusion that the fits presented in table 16 can be considered as the most accurate results. In addition to the non-universal constants given in the table and the universal amplitude ratio Q, this analysis yielded the (universal) irrelevant exponent $y_i = -0.82$ (3). This value is in very good agreement with that obtained by Nickel and Rehr [8]. Although there is one more unknown (y_i), the results for Q and K_c obtained in this section are more accurate than those of the three separate fits. One of the reasons is that the fit for model 3 is insensitive to the value of y_i, so that, e.g., Q is determined accurately.

Table 17. Some recent results for the renormalization exponents. The estimate for y_i from [3] has been calculated from the value for $\theta = -y_i/y_t$ presented in this reference and the value for y_t as calculated in the present work.

	Year	y_t	y_h	y_i
Present work	1995	1.587 (2)	2.4815 (15)	−0.82 (6)
Kolesik and Suzuki [11]	1995	1.586 (4)	2.482 (4)	
Guttman and Enting [10]	1994	1.580 (3)		
Landau [21]	1994	1.590 (2)	2.482 (7)	
Baillie *et al* [19]	1992	1.602 (5)	2.4870 (15)	−0.8 to −0.85
Nickel [9]	1991	1.587	2.4823	−0.84
Nickel and Rehr [8]	1990	1.587 (4)	2.4821 (4)	−0.83 (5)
Le Guillou and Zinn-Justin [2]	1980	1.587 (4)	2.485 (2)	−0.79 (3)

7. Discussion and conclusion

Let us summarize our final results for the renormalization exponents: $y_t = 1.587$ (2), $y_h = 2.4815$ (15), $y_i = -0.82$ (6). To allow for any residual dependences on the choice of the fitting formulae, we list error margins of two standard deviations. In table 17 we compare our results with some recent estimates obtained by various methods. Our result for the temperature exponent is lower than that of Baillie *et al* [19], obtained by the Monte Carlo renormalization method. This could be explained by a violation of hyperscaling. However, the accurate agreement between our result and that of coupling-constant expansion [2], ε-expansion [6], series expansions [8,9] and the coherent-anomaly method [11] makes this explanation less likely. We notice that our result for y_t is markedly higher than the recent series-expansion result of Guttman and Enting [10]. The result for the magnetic exponent is also in good agreement with most other estimates, although the result of Baillie *et al* lies significantly higher than the majority of the results. Also the result of Le Guillou and Zinn-Justin obtained by coupling-constant expansion [2] seems somewhat too high. The results for the leading irrelevant exponent are not very accurate, but consistent. We notice that the fractions $\frac{73}{46}$ and $\frac{67}{27}$ are good approximations for y_t and y_h, respectively. For easy reference, table 18 summarizes the exponents α, β, γ, δ, η, ν and θ as calculated from our results for y_t, y_h and y_i, on the assumption that the hypotheses of scaling and hyperscaling are valid.

Table 18. The standard critical exponents as well as Wegner's correction-to-scaling exponent θ as calculated from our best estimates for y_t, y_h and y_i.

Exponent	Expressed in RG exp.	Value
α	$2-d/y_t$	0.110 (2)
β	$(d-y_h)/y_t$	0.3267 (10)
γ	$(2y_h-d)/y_t$	1.237 (2)
δ	$y_h/(d-y_h)$	4.786 (14)
η	$2-2y_h+d$	0.037 (3)
ν	$1/y_t$	0.6301 (8)
θ	$-y_i/y_t$	0.52 (4)

Furthermore, we can calculate the Binder cumulant U from our estimate for Q, using the relation $U = 3 - 1/Q$, which yields $U = 1.3956$ (10). Only a few accurate results are available for this quantity (see, e.g., [45] for a review) and one of the most accurate estimates up till now is $U = 1.403$ (7) [46]. Our result is in agreement with this and other estimates, but its accuracy is markedly higher. We have not sampled the characteristic length ξ_L defined by Baker and Kawashima [47] in our simulations. Thus, we have no result for the renormalized coupling constant g^*, which differs from the Binder cumulant by a factor $(L/\xi_L)^d$ [47].

Table 19 presents a comparison of recent results for K_c of the spin-$\frac{1}{2}$ nearest-neighbour Ising model. Again, it should be noted that the error margin of the result obtained in the present work amounts to two standard deviations. It can be seen that the amplitude ratio Q, which is used in this work, provides a good means of obtaining an accurate estimate for the critical coupling. We conclude that the conjecture of Rosengren [48] is not correct. The result of Ferrenberg and Landau deviates by 1.8 combined standard errors, but the newest estimate of Landau differs by only 1.2 standard deviations from the result presented here. The difference with [20] is 1.6 standard errors and is partly due to statistical errors (the data

Table 19. Summary of recent results for the critical point of the spin-$\frac{1}{2}$ Ising model with nearest-neighbour couplings.

Reference	Year	Value
Present work	1995	0.221 6546 (10)
Landau [21]	1994	0.221 6576 (22)
Blöte and Kamieniarz [20]	1993	0.221 648 (4)
Baillie *et al* [19]	1992	0.221 652 (3)
Livet [36]	1991	0.221 6544 (10)
Ferrenberg and Landau [18]	1991	0.221 6595(26)
Ito and Suzuki [17]	1991	0.221 657 (3)
Blöte *et al* [14]	1989	0.221 652 (5)
Rosengren (conjecture) [48]	1986	0.221 6586(0)

used in this work include those of [20] but are much more accurate and include $L = 40$ data), and partly because a term with exponent y_2 was not included in the scaling formula for the ratio Q. Finally, we want to stress the importance of the spin-1 model. Since the corrections to scaling are small in this model, it is very suitable for the determination of universal quantities.

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Appendix. Experimental results

In this appendix, we have collected a number of experimental results for the various critical exponents of phase transitions which have been compared to results for the 3D Ising universality class. Only results published after 1980 are included. For binary mixtures, older results can be found in, e.g., [49]. The substances are grouped into four different subsets: unary systems, mixtures, magnetic systems and micellar systems (microemulsions). In general, the results agree very well with the theoretical values, but there are several remarkable discrepancies. Here, we only mention those measurements that differ by more than two standard deviations from our results. Results without error estimates are not taken into account.

The value for γ found in [70] lies much below the theoretical estimate. In [115] the results for both γ and ν do not appear to be Ising-like, as the authors have already noticed. The results for SF_6 presented in [63] are included, because the authors find mean-field values for the critical exponents, whereas the other results for the same substance appear to fall in the Ising universality class. For α, a range of values is found in [74], the lower end of which coincides with the theoretical value. In [105], two values of α are presented for MnF_2, 2.4σ above and 3.5σ below the theoretical value, respectively. Several very accurate results for the critical exponent β are presented in [57, 58, 66], which all lie much above the

Table A1. The various substances are grouped as follows: 'u' stands for unary systems, 'mx' for mixtures, 'mg' for magnetic systems and 'mi' for micellar systems (microemulsions). α, β, γ, δ and ν denote the standard critical exponents; θ is Wegner's correction-to-scaling exponent; the critical exponents which carry a tilde refer to Fisher's 'renormalized' critical exponents [50]. Abbreviations used: AOT = di-2-ethylhexylsulfosuccinate; BHDC = benzyldimethyl-*n*-hexadecylammoniumchloride; C_iE_j = $CH_3{\cdot}(CH_2)_{i-1}{\cdot}(O{\cdot}CH_2{\cdot}CH_2)_j{\cdot}OH$; HFC-32 = difluoromethane; HFC-125 = pentafluoroethene; R114 = $CClF_2{\cdot}CClF_2$; R13B1 = $CBrF_3$; R12 = CCl_2F_2; R22 = $CHClF_2$.

Substance	Type	Exponent	Value	Ref.
CO_2	u	α	0.111 (1)	[51]
		β	0.324 (2)	
Cs	u	α	0.13 (3)	[52]
		β	0.355 (10)	
Ethane	u	β	0.327 (2)	[53]
		θ	0.46 (4)	
Fluoroform	u	β	0.329 (1)	[54]
GeH_4	u	β	0.333 (8)	[55]
H_2	u	β	0.326 (3)	[56]
		γ	1.19 (5)	
		θ	0.46 (2)	
HD	u	β	0.352 (1)	[57]
HFC-32	u	β	0.345 (1)	[58]
HFC-125	u	β	0.341 (2)	[58]
Ne	u	β	0.3575 (10)	[57]
Ne, N_2	u	β	0.327 (2)	[59]
		θ	0.51 (3)	
		θ	0.49 (5)	
R114	u	β	0.312	[60]
R13B1	u	β	0.340	[61]
R12	u	β	0.337	[62]
R22	u	β	0.348	[62]
Rb	u	α	0.14 (3)	[52]
		β	0.36 (1)	
SF_6	u	β	0.48 (3)	[63]
		β	0.325 (5)	[64]
		β	0.338	[65]
		β	0.350 (4)	[66]
		β	0.355	[67]
		γ	0.98 (5)	[63]
		γ	1.24 (2)	[66]
		δ	3.0 (2)	[63]
1,1,1,2-tetrafluoroethane	u	β	0.340 (1)	[68]
Xe	u	γ	1.246 (10)	[69]
Methanol + hexane	mx	γ	1.09 (3)	[70]
		$\gamma - \alpha$	1.04(3)	
Methanol + cyclohexane	mx	β	0.33 (2)	[71]
		γ	1.26 (5)	[72]
		ν	0.64 (2)	
Methanol + *n*-heptane	mx	β	0.3337 (5)	[73]
		α	0.11–0.35	[74]
Methanol + isooctane	mx	β	0.323 (9)	[75]
n-hexane + *n*-tetradecafluorohexane	mx	β	0.35 (1)	[76]
Acetonitrile + cyclohexane	mx	β	0.322 (4)	[77]
Butylcellosolve + H_2O	mx	α	0.077 (41)	[78]
		β	0.319 (14)	
		γ	1.24 (1)	
		ν	0.606 (18)	

Table A1. (Continued)

Substance	Type	Exponent	Value	Ref.
Iso-butoxyethanol + H_2O	mx	α	0.105 (8)	[79]
Isobutyric acid + H_2O	mx	β	0.326 (3)	[80]
		γ	1.19 (21)	[81]
		ν	0.654 (9)	
Deuterated cyclohexane + cyclohexane + H_2O	mx	β	0.323 (3)	[82]
		β	0.326 (2)	
		β	0.322 (2)	
n,*n*-dimethylacetamide + octane	mx	β	0.324 (5)	[83]
		β	0.329 (2)	
n,*n*-dimethylacetamide + decane	mx	β	0.329 (4)	[84]
		β	0.333 (2)	
Ethylammoniumnitrate + *n*-octanol	mx	ν	0.610 (6)	[85]
Ethyleneglycolmonoisobutylether + H_2O	mx	β	0.332 (2)	[86]
2,6-lutidine + H_2O	mx	β	0.336 (30)	[87]
Nitroethane + cyclohexane, benzonitrile + isooctane	mx	β	0.325 (5)	[88]
Nitrobenzene + isooctane	mx	α	0.145 (35)	[89]
Nitrobenzene + decane + benzene	mx	$\tilde{\beta}$	0.376 (8)	[90]
Perfluoroheptane + CCl_4	mx	β	0.324 (5)	[91]
Triethylamine + H_2O	mx	θ	0.52 (3)	[92]
Triethylamine + H_2O + D_2O	mx	α	0.110 (4)	[93]
Trimethylethylammoniumbromide + chloroform	mx	ν	0.621 (3)	[94]
Tetrachloromethane + tetradecafluoromethylcyclohexane	mx	β	0.289 (6)	[95]
Tetra-*n*-pentylammoniumbromide + H_2O	mx	β	0.3370 (22)	[96]
		β	0.3190 (11)	
		β	0.3167 (16)	
CO_2 + *n*-butane	mx	β	0.359	[97]
		ν	0.66	
CO_2 + *n*-decane	mx	β	0.368	[98]
		ν	0.646	
Na + NH_3	mx	β	0.34 (1)	[99]
		θ	0.46 (3)	
Na + ND_3	mx	γ	1.228 (39)	[100]
		γ	1.2400 (157)	
		γ	1.223 (19)	
		η	0.0300 (15)	
		η	0.0317 (13)	[101]
		η	0.0302 (15)	
		ν	0.6279 (80)	[100]
CoF_2	mg	α	0.109 (6)	[102]
DyAlG	mg	β	0.33 (1)	[103]
$FeCl_2$	mg	α	0.15(4)	[104]
FeF_2	mg	α	0.111 (7)	[105]
		α	0.115 (4)	
		α	0.11 (3)	[106]
		β	0.325 (2)	[107]
		γ	1.25 (1)	[108]
$MnBr_2$	mg	α	0.118 (7)	[109]
$MnCl_2$	mg	β	0.297 (3)	[110]
MnF_2	mg	α	0.123 (5)	[105]
		α	0.091 (5)	
$NdRu_2Si_2$	mg	α	0.11 (3)	[111]
U_3P_4	mg	β	0.315 (15)	[112]
		β	0.313 (15)	
		γ	1.25 (2)	

Table A1. (Continued)

Substance	Type	Exponent	Value	Ref.
AOT + *n*-decane + H_2O	mi	γ	1.26 (10)	[113]
		γ	1.22 (5)	[114]
		γ	1.61 (9)	[115]
		ν	0.61 (6)	[113]
		ν	0.75 (5)	[114]
		ν	0.68 (8)	
		ν	0.72 (4)	[115]
Benzene + BHDC + H_2O	mi	β	0.34 (8)	[116]
		γ	1.18 (3)	[117]
		ν	0.60 (2)	[117]
2-butoxyethanol + D_2O	mi	γ	1.216 (13)	[118]
		η	0.039 (4)	
		ν	0.623 (13)	
C_6E_3 + H_2O	mi	α	0.11 (4)	[119]
		β	0.327 (4)	
		γ	1.24 (1)	
		γ	1.241 (16)	[120]
		η	0.016 (5)	[119]
		ν	0.627 (6)	
		ν	0.632 (11)	[120]
C_8E_4 + H_2O	mi	γ	1.237 (7)	[120]
		γ	1.243 (7)	
		ν	0.630 (12)	
		ν	0.630 (18)	
$C_{10}E_4$ + H_2O	mi	γ	1.25 (2)	[121]
		ν	0.63 (1)	
$C_{12}E_5$ + H_2O	mi	γ	1.17 (11)	[122]
		ν	0.65 (4)	
$C_{12}E_6$ + D_2O	mi	γ	1.2 (1)	[123]
		ν	0.60 (5)	
$C_{12}E_6$ + H_2O	mi	γ	1.2 (1)	[124]
		ν	0.60 (3)	
$C_{12}E_8$ + D_2O	mi	γ	1.21 (2)	[125]
		ν	0.62 (2)	
$C_{12}E_8$ + H_2O	mi	γ	1.20 (4)	[125]
		ν	0.63 (1)	
Sodiumdodecylsulphate + butanol + NaCl	mi	ν	0.62 (3)	[126]
		ν	0.64 (4)	
		ν	0.63 (5)	
Cationic surfactant in aqueous salt solution	mi	$\tilde{\beta}$	0.375 (10)	[127]
		$\tilde{\gamma}$	1.39 (4)	
		$\tilde{\nu}$	0.70 (3)	

result in table 18. On the other hand, the accurate results in [95, 110] lie much lower than the theoretical prediction. The differences in [52, 84, 86] are less severe, but all results in these references lie between 2 and 3 combined standard errors above the theoretical value. Also the results for β presented in [96] deviate by many standard errors from the theoretical value, although the authors of this reference state that they consider the differences as not significant. The authors of [73] found a good fit of their data to a value of $\beta = 0.3337$ (5), but conclude that this value is probably too high.

For ν, very low values have been found in [85, 94], whereas the value in [81] lies 2.6

standard errors above our result. In [119], the result $\eta = 0.016\ (5)$ is given, which deviates by about four combined standard deviations from the best theoretical values. Nevertheless, the authors of [119] consider it to be in good agreement.

In general, it is difficult to assess the source of the discrepancies noticed here, although there certainly are cases where crossover phenomena and corrections to scaling were not taken into account in the data analysis.

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