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The magnetization of the 3D Ising model

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Abstract. We present highly accurate Monte Carlo results for simple cubic Ising lattices containing up to 256^3 spins. These results were obtained by means of the Cluster Processor, a newly built special-purpose computer for the Wolff cluster simulation of the 3D Ising model. We find that the spontaneous magnetization $M(t)$ is accurately described by $M(t) = (a_0 - a_1 t^\theta - a_2 t)t^\beta$, where $t = (T_c - T)/T_c$, in a wide temperature range $0.0005 < t < 0.26$. Any corrections to scaling with higher powers of t could not be resolved from our data, which implies that they are very small. The magnetization exponent is determined as $\beta = 0.3269(6)$. An analysis of the magnetization distribution near criticality yields a new determination of the critical point: $K_c = J/k_B T_c = 0.221\,6544$, with a standard deviation of 3×10^{-7}.

We consider the 3D Ising model on the simple cubic lattice, with nearest-neighbour interactions J, at a temperature T and a coupling strength $K = J/k_B T$. At criticality, the spontaneous magnetization vanishes with a singularity $M(t) \propto t^\beta$, where $t = (T_c - T)/T_c = (K - K_c)/K$ parametrizes the distance to the critical point. However, this law applies only in the limits of infinite system size and $t \to 0$. Even for the infinite system there are corrections due to non-zero values of t:

$$M(t) = f_t(t) t^\beta \tag{1}$$

where f_t is some function of t, finite at $t = 0$.

For the 2D Ising model this function is known exactly, and it is analytic. However, in the 3D case, f_t is not analytic at $t = 0$. The leading terms of its expansion near $t = 0$ are

$$f_t(t) \approx a_0 - a_1 t^\theta \tag{2}$$

where $\theta \approx 0.5$ is Wegner's correction-to-scaling exponent [1].

Generally one would expect that there exist many more terms, containing higher powers of t, in the expansion of f_t. Quite remarkably, we find that it is sufficient to add only one term, $-a_2 t$, to equation (2), in order to describe $M(t)$ of the simple cubic 3D Ising model with very high accuracy. This does not only apply close to $t = 0$; it holds in a wide range of t.

We found this intriguing fact using the Cluster Processor (CP) [2]. The CP implements the cluster Wolff algorithm [3] in hardware, for 3D simple cubic Ising models with nearest-neighbour interactions and periodic boundaries. Its memory and speed are sufficient to simulate Ising systems containing up to 256^3 spins. The CP was checked to give correct results for 2D Ising systems. Moreover the CP data are also consistent with earlier very

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accurate simulations on 16^3 and 32^3 lattices [4]. In the CP, the system size can take the five values 16, 32, 64, 128, 256 along each spatial direction. But the present work is restricted to systems with the same size L in all three directions.

To determine f_t, one should eliminate the influence of the finite system size. This can be easily achieved by a comparison of data for different sizes. The corrections due to finite L can be described by a scaling function f_L:

$$M(t) = f_L(Lt^{\nu})t^{\beta} \tag{3}$$

where the exponent ν describes the divergence of the correlation length when the critical temperature is approached. The relation (3) is valid in the limit $t \to 0$. The argument of the function f_L is proportional to the ratio of the finite size and the correlation length. Thus, f_L is expected to be a constant for large values of its argument.

The meaning of $M(t)$ in equation (3) has to be made more precise, since the average magnetization of a finite system vanishes. Instead, we may define a non-zero expectation value in terms of the absolute value of M:

$$M_m = \langle |M| \rangle. \tag{4}$$

We can also find $M(t)$ from the spin–spin correlation function, using the relation $M^2 = \langle S(0)S(\infty)\rangle$. For a finite lattice this infinite distance can be replaced by $L/2$, half way to the periodic images of the spins. Therefore we use the following expression as the second definition of the magnetization:

$$M_c = \langle S(0)S(L/2)\rangle^{1/2}. \tag{5}$$

Finally, the magnetization can be defined as $M_2 = \langle M^2\rangle^{1/2}$. This quantity has been studied in [5] for the 2D Ising model and in [6] for the 3D case. In agreement with [5, 6] we found that M_2 is strongly affected by finite-lattice effects even for large t, so we do not use M_2 in this paper.

The scaling functions f_L are different for M_m and M_c. This helps determine the ranges of t where the finite-size effects become important.

Our data show, that for a given L, the finite-size corrections to M_m and M_c are smaller than the error bars for $t > t_L$. For $L = 32$ this is illustrated by figure 1, which clearly demonstrates that M_m and M_c coincide for $t > t_{32}$, and t_{32} is about 1.5×10^{-2}. From figure 1 one can see that for t just below t_L the corrections to M_m and M_c have different signs, which facilitates determination of t_L.

The value of t_L can be estimated in the following way. The finite-lattice effects become important when the correlation length $\xi \propto t^{-\nu}$ is comparable with L. Therefore

$$at_L^{-\nu} = L \tag{6}$$

where a is a numerical coefficient. Taking into account $\nu = 0.63$ [4], we get $a \approx 2$, which seems reasonable. According to equation (6), a doubling of L decreases t_L by a factor $2^{1/\nu} \approx 3$. This is in agreement with figure 2, which shows the normalized $M_m(t)$ results for three different lattice sizes.

To study $f_t(t)$ we used data for lattice sizes ranging from 32^3 to 256^3. Only data for $t > t_L$, where M_m and M_c coincide, were taken into account. The results for $M(t)$ are shown in figure 3, using a logarithmic scale on both axes. Close to the critical point, for $t < 0.02$, the plot seems to be linear. However, attempts to approximate the data by $t^{\beta}P(t)$, where $P(t)$ is an arbitrary polynomial in t, were not successful. Figure 4 shows the poor result of such an attempt. It describes the ratio of the simulation data to

$$M_{\text{int}}(t) = t^{\beta}(p_0 + p_1 t + p_2 t^2 + p_3 t^3). \tag{7}$$

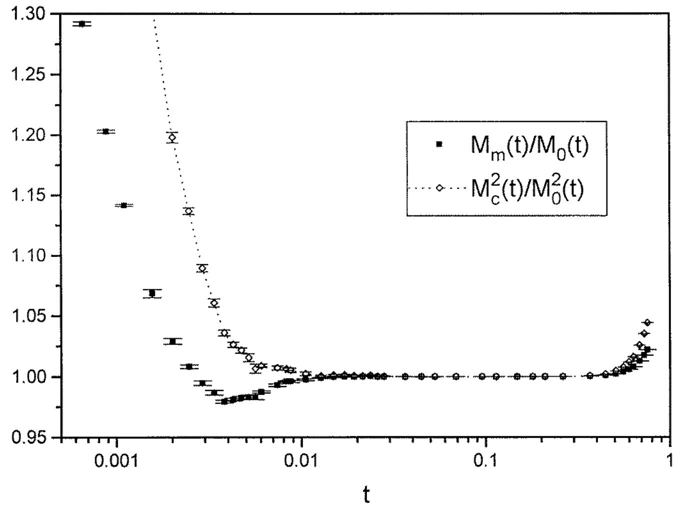

Figure 1. Normalized magnetization $M_m(t)$ and the correlation function $\langle S(0)S(L/2)\rangle \equiv M_c^2$ for the 32^3 lattice. $M_0(t)$ is given by equation (9). The normalization makes it possible to expand the scale so that the small deviations of $M(t)$ from $M_0(t)$ become visible. $\langle S(0)S(L/2)\rangle$ is close to $M_0^2(t)$, and $M(t)$ is close to $M_0(t)$ for $t > t_{32} \approx 0.015$. For $t > 0.26$ the deviations of the CP data from $M_0(t)$ grow rapidly. In this low-temperature range the simulation data are in excellent agreement with the Padé approximant of [9].

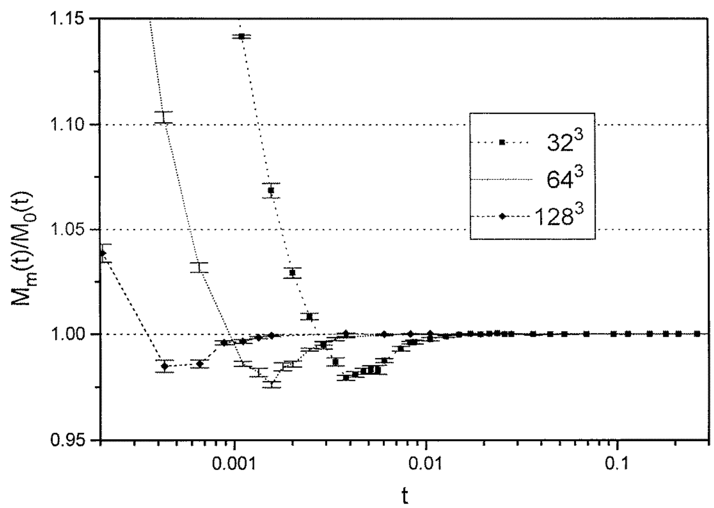

Figure 2. Normalized magnetization $M_m(t)$ for three different lattice sizes $L = 32$, 64, and 128. The small-t behaviour displays the characteristics of the finite-size scaling function f_L associated with M_m.

The exponent β and the coefficients p_i were determined by the least-squares method, in order to describe the simulation data as closely as possible by equation (7). Nevertheless, the differences between the CP data and the approximation by equation (7) are much larger than the error bars.

This suggests that we should use the form equation (2) instead to describe $f_t(t)$. Thus

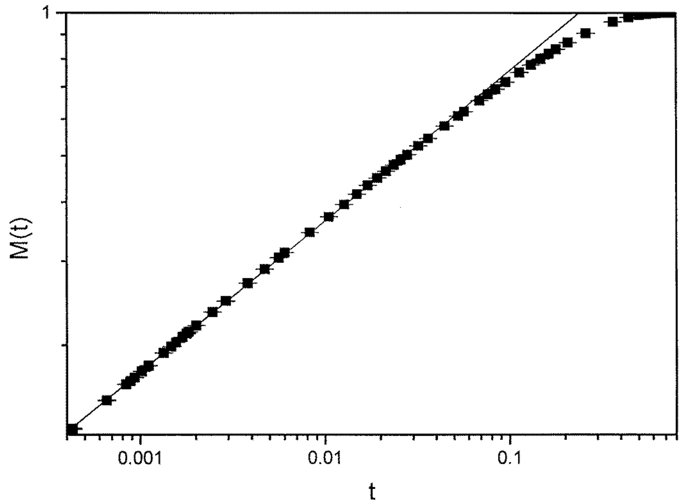

Figure 3. Spontaneous magnetization of the 3D Ising model as a function of t, with a logarithmic scale on both axes. The statistical errors in these data points are indicated, but they appear only as single horizontal bars, because the errors are below the resolution of this figure. The data shown here apply to different lattice sizes, and were taken in those ranges of t where finite-lattice effects are negligible: they describe the infinite system magnetization.

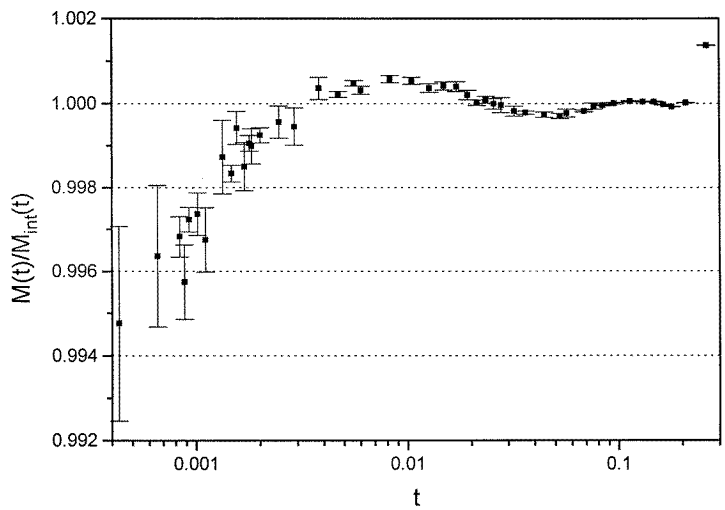

Figure 4. Ratio of magnetization data to the approximation $M_{\mathrm{int}}(t)$ given in equation (7), where the function $f_t(t)$ was supposed to contain only integer powers of t. This figure demonstrates that, without the Wegner correction to scaling, even a five-parameter fit according to equation (7) does not describe the CP data properly. In this equation we used the same number of adjustable parameters as in $M_0(t)$ (see equation 9), but, as can be seen by comparing figures 4 and 5, the latter approximation is far better.

we wrote $f_t(t)$ as a polynomial in $t^{1/2}$

$$f_{t1} = a_0 - a_1 t^{1/2} - a_2 t. \tag{8}$$

Even the first attempt to approximate the simulation data as $t^{\beta} f_{t1}$ with $\beta = 0.3267$, taken

Table 1. Results of least-square fits of the magnetization data obtained by the CP. These fits were made for three choices of the critical coupling K_c.

K_c	β	θ	a_0	a_1	a_2	χ^2
0.221 6544	0.3269(3)	0.508(15)	1.692(4)	0.344(6)	0.426(11)	0.844
0.221 6541	0.3274(3)	0.490(15)	1.698(4)	0.340(5)	0.436(10)	0.859
0.221 6547	0.3265(3)	0.528(15)	1.686(4)	0.348(7)	0.414(12)	0.848

from [4], and a_0, a_1, a_2 regarded as free parameters, was very successful. But the high statistical accuracy of the CP data allows the use of even more adjustable parameters, and we supposed that the magnetization can be described by

$$M_0(t) = (a_0 - a_1 t^\theta - a_2 t)t^\beta \tag{9}$$

in the interval $0.26 > t > 0.0005$. The five parameters β, θ and a_i were determined by a nonlinear least-squares fit. To estimate the influence of the uncertainty in K_c, we fitted the parameters not only for our best estimate $K_c = 0.221\,6544$ (see below), but also for the lower and upper limits of K_c, defined by one standard deviation (3×10^{-7}) of the critical coupling. The results are shown in table 1. The last column characterizes the quality of the least-squares approximation. It is defined as

$$\chi^2 = \frac{1}{N-n}\sum_{i=1}^{N}\left(\frac{M(t_i) - M_0(t_i)}{\sigma(t_i)}\right)^2$$

where $n = 5$ is the number of fitted parameters, $N = 45$ is the number of magnetization data points, and the $\sigma(t_i)$ are the standard deviations of the magnetization data $M(t_i)$. The minimum of χ^2 as a function of K appears to occur near $K_c = 0.221\,6544$ as determined from an analysis of the magnetization distribution near the critical point (see below). This agreement between two different approaches suggests that our scaling formulae are adequate.

From the data in the second column we estimate the magnetization exponent as $\beta = 0.3269(6)$, which is in a good agreement with earlier values, see e.g. [4] and references therein.

The third column indicates that $\theta = 0.508(25)$, supporting earlier results obtained by means of an ϵ-expansion analysis [7], series expansions [8] and a finite-size scaling analysis of three different Ising models [4].

It should be emphasized that the errors in the parameters in table 1 are strongly correlated; thus, equation (9) represents the magnetization data much more accurately than one might naively expect from the quoted standard errors. In order to do justice to the accuracy of this representation, we rewrite equation (9) using several additional decimal places:

$$M_0(t) = t^{0.326\,941\,09}(1.691\,9045 - 0.343\,577\,31 t^{0.508\,420\,26} - 0.425\,723\,66 t) \tag{10}$$

where $t = 1 - 0.221\,6544 k_B T/J$. This formula may serve as a very accurate empirical approximation for the spontaneous magnetization of the simple cubic Ising model in the region $0.26 > t > 0.0005$.

In the range of t between 0.24 and 0.17, the results of equation (10) numerically coincide with the Padé approximant of [9] within 10^{-5}, while for smaller t the approximation (10) is superior.

The ratio of the CP data to $M_0(t)$ is shown in figure 5. The simulation data coincide with $M_0(t)$ within the error bars. No systematic deviation of the CP data from $M_0(t)$ can be found.

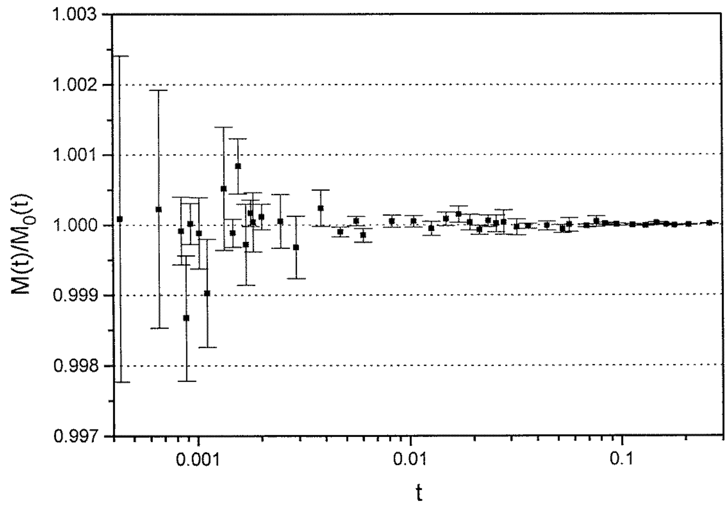

Figure 5. Normalized magnetization data, describing the infinite 3D Ising system. This figure demonstrates that the expression equation (9) for $M(t)$ agrees with the simulation data within the statistical errors. The relative accuracy of the formula is as high as 10^{-3} for $t \approx 10^{-3}$, and better than 10^{-4} for $t > 0.01$. This picture combines all the magnetization data, obtained with different precisions and for different lattice sizes. Long simulation times were required for some of these points in order to obtain such small error bars.

Table 2. Numerical results for the dimensionless ratio $Q_L = \langle m^2 \rangle_L^2 / \langle m^4 \rangle_L$ for finite three-dimensional Ising models close to the critical point. Also shown is the total number of Wolff clusters flipped by the CP to obtain each numerical result.

L	K	Q_L	Number of clusters
16	0.221 6530	0.633 81(5)	1×10^9
32	0.221 6530	0.628 83(10)	3×10^8
64	0.221 6530	0.624 69(79)	2.5×10^7
64	0.221 6545	0.626 70(25)	2.5×10^8
128	0.221 6530	0.621 89(168)	1×10^7
128	0.221 6545	0.626 03(84)	4×10^7
256	0.221 6530	0.615 55(180)	2.6×10^7

The function f_t may also contain a term proportional to $t^{2\theta}$. Because θ is very close to 0.5, the simulation accuracy is not sufficient to distinguish the term $(a_2 t)$ in equation (9) from the sum $(a_{21} t + a_{22} t^{2\theta})$.

The CP was also used for some additional calculations close to the critical point. We obtained the dimensionless ratio $Q = \langle m^2 \rangle^2 / \langle m^4 \rangle$, related to the Binder cumulant [10]. The Q values are shown in table 2.

These data were combined with those available from [4] in order to determine the critical point more accurately. Near T_c, the bulk correlation length satisfies $\xi \gg L$, so that Lt^{ν}, and hence $(K - K_c)L^{y_t}$, is small. Thus $Q_L(K)$ can be expanded as

$$Q_L(K) = Q + q_1(K - K_c)L^{y_t} + q_2(K - K_c)^2 L^{2y_t} + b_1 L^{y_i} + b_2 L^{y_2}. \qquad (11)$$

The renormalization exponents y_t and y_i are related to ν and θ as $y_t = \nu^{-1}$ and $y_i = -\theta/\nu$. The substitutions of the values $y_t = 1.587(2)$, $y_i = -0.82(6)$ and $y_2 = -1.963(3)$, taken from [4], into equation (11) was found to describe the combined data satisfactorily. A least-squares fit was used to determine K_c. For system sizes $L \geqslant 5$ the same fit as in [4] yielded $K_c = 0.221\,6544(3)$, where the standard error includes the uncertainty in the input parameters. As a final estimate we quote $K_c = 0.221\,6544(6)$ with an error of two standard deviations, in order to account for a possible bias introduced by our choice of the form of equation (11). The additional data in table 2 permitted a clear improvement of the accuracy in comparison with [4]. This new value for the Ising critical point is in a good agreement with a number of recent results obtained by several other methods, such as series expansions and Monte Carlo renormalization. These results are summarized e.g. in [11] and [4].

We calculated the irrelevant exponent y_i in two ways. First, it can be obtained as a product of $\theta = 0.508(25)$, found from table 1, and $y_t = 1.587(2)$ [4]. The result is $y_i = -0.81(4)$. Another possibility is to include y_i as a free parameter in the $Q_L(K)$ fitting procedure. This yields $y_i = -0.83(9)$, in agreement with the result obtained above. Our values for y_i agree with the ϵ-expansion [7] as well as with other results, see e.g. [4] and references therein.

Furthermore, we have combined the new data for $\langle m^2 \rangle$ near the critical point with those obtained in [4] for the nearest-neighbour model with system sizes up to $L = 40$. The analysis was based on the expected scaling behaviour of the susceptibility (see [4])

$$L^d \langle m^2 \rangle = c_0 + c_1(K - K_c) + \cdots \\ + L^{2y_h - d}[d_0 + d_1(K - K_c)L^{y_t} + d_2(K - K_c)L^{2y_t} + g_1 L^{y_i} + g_2 L^{2y'}]$$

with $K_c = 0.221\,6544$ and $y' = -2.1$. The renormalization exponent y_h is related to the magnetic susceptibility critical exponent γ: $2y_h - d = \gamma/\nu$. The analysis for $L \geqslant 5$ yielded $y_h = 2.4808(16)$ where we again quote a two-sigma error. This result is in good agreement with [4] and references therein, and with [12].

Acknowledgments

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