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Nonmonotonic external field dependence of the magnetization in a finite Ising model: Theory and MC simulation

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Abstract. Using φ^4 field theory and Monte Carlo (MC) simulation we investigate the finite-size effects of the magnetization M for the three-dimensional Ising model in a finite cubic geometry with periodic boundary conditions. The field theory with infinite cutoff gives a scaling form of the equation of state $h/M^\delta = f(hL^{\beta\delta/\nu}, t/h^{1/\beta\delta})$ where $t = (T - T_c)/T_c$ is the reduced temperature, h is the external field and L is the size of system. Below T_c and at T_c the theory predicts a nonmonotonic dependence of $f(x, y)$ with respect to $x \equiv hL^{\beta\delta/\nu}$ at fixed $y \equiv t/h^{1/\beta\delta}$ and a crossover from nonmonotonic to monotonic behaviour when y is further increased. These results are confirmed by MC simulation. The scaling function $f(x, y)$ obtained from the field theory is in good quantitative agreement with the finite-size MC data. Good agreement is also found for the bulk value $f(\infty, 0)$ at T_c.

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1 Introduction

The scaling equation of state near a critical point provides fundamental information on the critical behaviour of a thermodynamic system. For bulk Ising-like systems accurate predictions have been made recently [1] on the basis of the φ^4 field theory in three dimensions. Testing these predictions by Monte Carlo simulations [2] would be of considerable interest. Such simulations, however, are necessarily made only for finite systems and thus phenomenological concepts like finite-size scaling [3] are needed to perform extrapolations from mesoscopic lattices.

In order to test the theory in a more conclusive way it is desirable to go beyond the phenomenological finite-size scaling concept and to calculate explicitly the finite-size effects on the equation of state, *i.e.*, on the magnetization as a function of the temperature T and external field h in a finite geometry. Although such field-theoretic calculations [4–7] are perturbative and not exact they have been found to be in good agreement with the MC simulations. So far the calculations of thermodynamic quantities were restricted to the case of zero external field h. At finite h, only the order-parameter distribution function was calculated [8–10]. In the present paper we extend these calculations to the equation of state of the three-dimensional Ising model in a finite cubic geometry at finite h. For simplicity these calculations are performed at infinite cutoff and thus our results neglect lattice effects. The latter have been shown [11–13] to yield non-negligible contributions to the exponential part of the finite-size scaling function. Here we focus our interest on the universal scaling part of the equation of state. Our theory predicts non-monotonic effects in the h dependence of the equation of state which we then confirm with surprisingly good agreement by standard Monte Carlo simulations.

The identification of such non-monotonic effects is of great practical importance. If, for example, the characteristic temperature $T_c(L)$ of a lattice with L^3 sites in three dimensions varies asymptotically as $T_c(L) - T_c(\infty) \propto 1/L^y$ with some correlation length exponent $y = 1/\nu$, then a plot of the numerical $T_c(L)$ *versus* $1/L^y$ gives the extrapolated $T_c(\infty)$ as an intercept. If, however, higher order terms make the curve $T_c(L)$ non-monotonic, then such a plot for finite L, where the non-monotonicity is not yet visible, would give a wrong estimate for $T_c(\infty)$. Similar effects would make estimates of other quantities unreliable, and there exist examples of such estimates in the literature.

2 Field-theoretic calculations

We consider the φ^4 model with the standard Landau-Ginzburg-Wilson Hamiltonian

$$H(h) = \int_V \left[\frac{1}{2} r_0 \varphi^2 + \frac{1}{2}(\bigtriangledown\varphi)^2 + u_0 \varphi^4 - h\,\varphi\right] \qquad (1)$$

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where $\varphi(\mathbf{x})$ is a one-component field in a finite cube of volume $V = L^d$ and h is a homogeneous external field. We assume periodic boundary conditions. Accordingly we have

$$\varphi(\mathbf{x}) = L^{-d} \sum_{\mathbf{k}} \varphi_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \tag{2}$$

where the summation $\sum_{\mathbf{k}}$ runs over discrete $\mathbf{k} = \frac{2\pi}{L}\mathbf{m}$ vectors with components $k_j = \frac{2\pi}{L} m_j, m_j = 0, \pm1, \pm2, ..., j = 1, 2, ..., d$ in the range $-\Lambda \le k_j < \Lambda$, *i.e.*, with a sharp cutoff Λ. The temperature enters through $r_0 = r_{0\mathrm{c}} + a_0 t, t = (T - T_\mathrm{c})/T_\mathrm{c}$.

As pointed out recently [11,12] the Hamiltonian (1) for periodic boundary conditions with a sharp cutoff Λ does not correctly describe the exponential size dependence of physical quantities of finite lattice models in the region $\xi \gg L$. Instead of (1), a modified continuum Hamiltonian with a smooth cutoff [12] would be more appropriate. Even better would be to employ the lattice version of the φ^4 theory to describe the lattice effect on the finite-size scaling variable of finite Ising models in the region $L > \xi$. In the present paper, however, we shall neglect such effects by taking the limit $\Lambda \to \infty$ (see below).

The fluctuating homogeneous part of the order-parameter of the Hamiltonian (1) is $\Phi = V^{-1}\int_V \mathrm{d}^d x \varphi(\mathbf{x}) = L^{-d}\varphi_0$. As previously [4,5] φ is decomposed as

$$\varphi(\mathbf{x}) = \Phi + \sigma(\mathbf{x}) \tag{3}$$

where $\sigma(\mathbf{x})$ includes all inhomogeneous modes

$$\sigma(\mathbf{x}) = L^{-d} \sum_{\mathbf{k}\neq\mathbf{0}} \varphi_{\mathbf{k}}\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}. \tag{4}$$

The order-parameter distribution function $P(\Phi) \equiv P(\Phi, t, h, L)$ is defined by functional integration over σ,

$$P(\Phi, t, h, L) = Z(h)^{-1} \int \mathrm{D}\sigma\, \mathrm{e}^{-H(h)}, \tag{5}$$

where

$$Z(h) = \int_{-\infty}^{\infty} \mathrm{d}\Phi \int \mathrm{D}\sigma\, \mathrm{e}^{-H(h)} \tag{6}$$

is the partition function of system. This distribution function depends also on the sharp cutoff Λ which implies non-scaling finite-size effects [11,12]. From the order-parameter distribution function $P(\Phi)$ we can calculate the magnetization

$$M = \langle|\Phi|\rangle = \int_{-\infty}^{\infty} \mathrm{d}\Phi\, |\Phi| P(\Phi). \tag{7}$$

The functional integration over σ in equations (5, 6) can only be done perturbatively [4–6]. Recently a novel approach was presented [7,8]. The main idea of this approach is to extend the non-perturbative treatment of the $\mathbf{k} = \mathbf{0}$ mode Φ [4–6] to all modes $\sigma_{\mathbf{k}}$ with $\mathbf{k} \neq \mathbf{0}$. This implies a non-perturbative treatment of the $\mathbf{k} \neq \mathbf{0}$ modes with non-Gaussian integrations over $\sigma_{\mathbf{k}}$ for each $\mathbf{k} \neq \mathbf{0}$. Using this approach the bare order-parameter distribution has been derived previously at finite h (see (12-18) of Ref. [8]) for general n where n is the number of components of the order-parameter.

In the present case ($n = 1$) the result can be written in the form

$$P(\Phi) = \mathrm{e}^{-H^{\mathrm{eff}}(\Phi)} / \int_{-\infty}^{\infty} \mathrm{d}\Phi\, \mathrm{e}^{-H^{\mathrm{eff}}(\Phi)} \tag{8}$$

where the (bare) effective Hamiltonian of the Ising-like system reads

$$H^{\mathrm{eff}}(\Phi) = H_0(\Phi, h) - \frac{1}{2} \sum_{\mathbf{m}\neq\mathbf{0}} \ln\left\{\frac{Z_1[y_{0\mathbf{m}}(r_{0L})]}{Z_1[y_{0\mathbf{m}}(r_0)]}\right\}, \tag{9}$$

$$H_0(\Phi, h) = L^d(\frac{1}{2} r_0 \Phi^2 + u_0 \Phi^4 - h\,\Phi), \tag{10}$$

with $r_{0L} = r_0 + 12u_0\Phi^2$ and $y_{0\mathbf{m}}(r) = (2L^d/3u_0)^{1/2}(r + \frac{4\pi^2}{L^2}\mathbf{m}^2)$. The function $Z_1[y]$ in equation (9) is defined as

$$Z_1[y] = \int_0^{\infty} \mathrm{d}s\; s \exp(-\frac{1}{2} y s^2 - s^4). \tag{11}$$

The non-Gaussian contributions enter *via* the the s^4 term of $Z_1[y]$. Their contributions to averages such as M vanish in the bulk limit $L \to \infty$ above T_c ($y > 0$) but stabilize $P(\Phi)$ below T_c ($y < 0$). In the both limits our order-parameter distribution function $P(\Phi)$ becomes equivalent to a one-loop approximation. At finite L, however, $P(\Phi)$ provides a smooth interpolation between the one-loop results below and above T_c. Our previous experience and comparison with Monte Carlo data at $h = 0$ [6,7] and $h \neq 0$ [8] shows that the renormalized form of $P(\Phi)$ in equations (12-22) below has good accuracy.

At this stage of the bare theory the h dependence enters only *via* the term $h\,\Phi$ in H_0, (10). In the renormalized form of $P(\Phi)$ (to be presented in (12-22) below) the h dependence will also enter through the h dependent choice of the flow parameter. Application of (7-11) to the critical region requires to renormalize the bare results. Using minimal renormalization at fixed dimension $d < 4$ [14] in the limit $\Lambda \to \infty$, we have previously derived the finite-size scaling form of the order-parameter distribution function for general n [7] at finite h [8]. In the present case ($n = 1$) the previous result (see Eqs. (34-36) of Ref. [8]) is reduced to

$$P(\Phi, t, h, L) = L^{\beta/\nu} p(hL^{\beta\delta/\nu}, tL^{1/\nu}, \Phi L^{\beta/\nu}), \tag{12}$$

where

$$p(x, q, z) = \frac{\exp[-F(x, q, z)]}{\displaystyle\int_{-\infty}^{\infty} \mathrm{d}z \exp[-F(x, q, z)]}, \tag{13}$$

with $x = hL^{\beta\delta/\nu}$, $q = tL^{1/\nu}$, $z = \Phi L^{\beta/\nu}$ and

$$F(x,q,z) = c_2(x,\hat{q})\hat{z}^2 + c_4(x,\hat{q})\hat{z}^4 - x\,z - \frac{1}{2}\sum_{\mathbf{m}\neq\mathbf{0}} \ln\left\{\frac{Z_1[y_{\mathbf{m}}(\tilde{r}_L(x,\hat{q},\hat{z}))]}{Z_1[y_{\mathbf{m}}(\tilde{r}_L(x,\hat{q},0))]}\right\}. \quad (14)$$

Here $\hat{q} = Q^* t(L/\xi_0)^{1/\nu}$ and $\hat{z} = (2Q^*)^\beta(\Phi/A_M)(L/\xi_0)^{\beta/\nu}$ are dimensionless variables normalized by the asymptotic amplitudes ξ_0 and A_M of the bulk correlation length $\xi = \xi_0 t^{-\nu}$ at $h=0$ above T_c and of the bulk order-parameter $M_{\mathrm{bulk}} = A_M|t|^\beta$ at $h=0$ below T_c. The bulk parameter Q^* is known [14]. The coefficients $c_2(x,\hat{q})$ and $c_4(x,\hat{q})$ read for $d=3$ (see Eqs. (40, 41) of Ref. [8] for $n=1$)

$$c_2(x,\hat{q}) = (64\pi u^*)^{-1}\hat{q}\tilde{\ell}(x,\hat{q})^{3-(2\beta+1)/\nu}(1+12u^*), \quad (15)$$

$$c_4(x,\hat{q}) = (256\pi u^*)^{-1}\tilde{\ell}(x,\hat{q})^{3-4\beta/\nu}(1+36u^*), \quad (16)$$

where u^* is the fixed point value of the renormalized coupling [14]. In three dimensions we have (see Eqs. (37, 38) of Ref. [8])

$$y_{\mathbf{m}}(\tilde{r}_L(x,\hat{q},\hat{z})) = [6\pi u^*\tilde{\ell}(x,\hat{q})]^{-1/2}[\tilde{r}_L(x,\hat{q},\hat{z})\tilde{\ell}(x,\hat{q})^2 + 4\pi^2\mathbf{m}^2], \quad (17)$$

$$\tilde{r}_L(x,\hat{q},\hat{z}) = \hat{q}\tilde{\ell}(x,\hat{q})^{-1/\nu} + (3/2)\tilde{\ell}(x,\hat{q})^{-2\beta\nu}\hat{z}^2. \quad (18)$$

The auxiliary scaling function $\tilde{\ell}(x,\hat{q})$ of the flow parameter is determined implicitly by (see Eqs. (42, 43) of Ref. [8])

$$\tilde{\ell}(x,\hat{q})^{3/2} = (4\pi u^*)^{1/2}[\tilde{y}(x,\hat{q}) + 12\vartheta_2(\tilde{y}(x,\hat{q}),\hat{x})], \quad (19)$$

$$\tilde{y}(x,\hat{q}) = (4\pi u^*)^{-1/2}\tilde{\ell}(x,\hat{q})^{3/2-1/\nu}\hat{q}, \quad (20)$$

$$\hat{x} = A_M(2Q^*)^{-\beta}\xi_0^{\beta/\nu}(4\pi u^*)^{1/4}\sqrt{8}\tilde{\ell}(x,\hat{q})^{\beta/\nu-3/4}x, \quad (21)$$

where

$$\vartheta_2(\tilde{y},\hat{x}) = \frac{\int_0^\infty \mathrm{d}s\; s^2\cosh(\hat{x}s)\exp(-\frac{1}{2}\tilde{y}s^2 - s^4)}{\int_0^\infty \mathrm{d}s\cosh(\hat{x}s)\exp(-\frac{1}{2}\tilde{y}s^2 - s^4)}. \quad (22)$$

The latter equation is the reduced form of equation (27) of reference [8] for $n=1$. The h dependence of $P(\Phi,t,h,L)$ enters explicitly *via* the term $-x\,z$ in (14) and implicitly (*via* the x dependence of c_2, c_4 and $\tilde{r}_L$) through the x dependence of the scaling function $\tilde{\ell}(x,\hat{q})^{3/2}$, (19), of the flow parameter. For a discussion of the appropriate choice of the flow parameter see reference [8]. From equations (7, 12) we obtain the scaling form

$$M(h,t,L) = L^{-\beta/\nu}f_M(hL^{\beta\delta/\nu}, tL^{1/\nu}), \quad (23)$$

$$f_M(x,q) = \frac{\int_{-\infty}^{\infty}\mathrm{d}z|z|\exp[-F(x,q,z)]}{\int_{-\infty}^{\infty}\mathrm{d}z\exp[-F(x,q,z)]}. \quad (24)$$

Correspondingly the asymptotic equation of state for a finite Ising-like system in the limit of zero lattice spacing [12] can be written as

$$h/M^\delta = f(hL^{\beta\delta/\nu}, t/h^{1/\beta\delta}) \quad (25)$$

where

$$f(x,y) = x/f_M(x, yx^{1/\beta\delta})^\delta. \quad (26)$$

In the comparison with the MC data of the simple-cubic (sc) Ising model in Section 4, the quantities h, M and L are used in a dimensionless form in units of the lattice constant (see Sect. 4 of Ref. [9]). We have taken the bulk parameters $u^* = 0.0412, Q^* = 0.945$ from reference [6]. From reference [15] we have taken the bulk amplitudes $\xi_0 = 0.495, A_M = 1.71$ in units of the lattice constant (of the sc Ising model) and the bulk critical exponents $\beta = 0.3305, \nu = 0.6335$. Thus our determination of the scaling function $f(x,y)$ does not require a new adjustment of nonuniversal parameters.

Taking the limit $hL^{\beta\delta/\nu} \to \infty$ at fixed $t/h^{1/\beta\delta}$, we obtain the scaling form of the bulk equation of state

$$h/M^\delta = f_\mathrm{b}(t/h^{1/\beta\delta}) = f(\infty, t/h^{1/\beta\delta}). \quad (27)$$

At $T = T_\mathrm{c}$ we find from equations (23-27)

$$h/M^\delta \equiv D_\mathrm{c} = f(\infty,0) = 0.202 \quad (28)$$

in three dimensions (in units of the lattice constant). In the subsequent sections our theoretical predictions will be compared with MC data for the three-dimensional Ising model.

3 Monte Carlo simulation

Standard heat bath techniques were used for the Glauber kinetic Ising model, with multi-spin coding (16 spins in each 64-bit computer word). Since the effect could be seen best in lattices of intermediate size $L \simeq 80$ for $L \times L \times L$ spins, memory requirements were tiny and only trivial parallelization by replication, not by domain decomposition, was used. However, thousands of hours of processor time were needed in order for us to see the non-monotonic effects clearly in our figure if h/M^δ is plotted. The exponent δ is nearly five and thus five percent accuracy in h/M^δ requires one percent accuracy in the directly simulated magnetization M.

In earlier simulations by the same author and algorithm [16] possible non-monotonic effects at $T = T_\mathrm{c}$ were not noticed because these simulations were primarily performed to study the bulk behaviour; at that time the field-theoretical predictions presented above were not yet known. But even if they had been known it is doubtful that with the Intel Paragon used in [16] instead of the Cray-T3E now the non-monotonic trends would have been seen in about the same computer time.

Because of the limited system size, errors in the magnetization of order $1 + \mathrm{const}/L^{\beta/\nu} \simeq 1 + \mathrm{const}/\sqrt{L}$ are expected; in light of these errors the agreement to be presented now is surprisingly good.

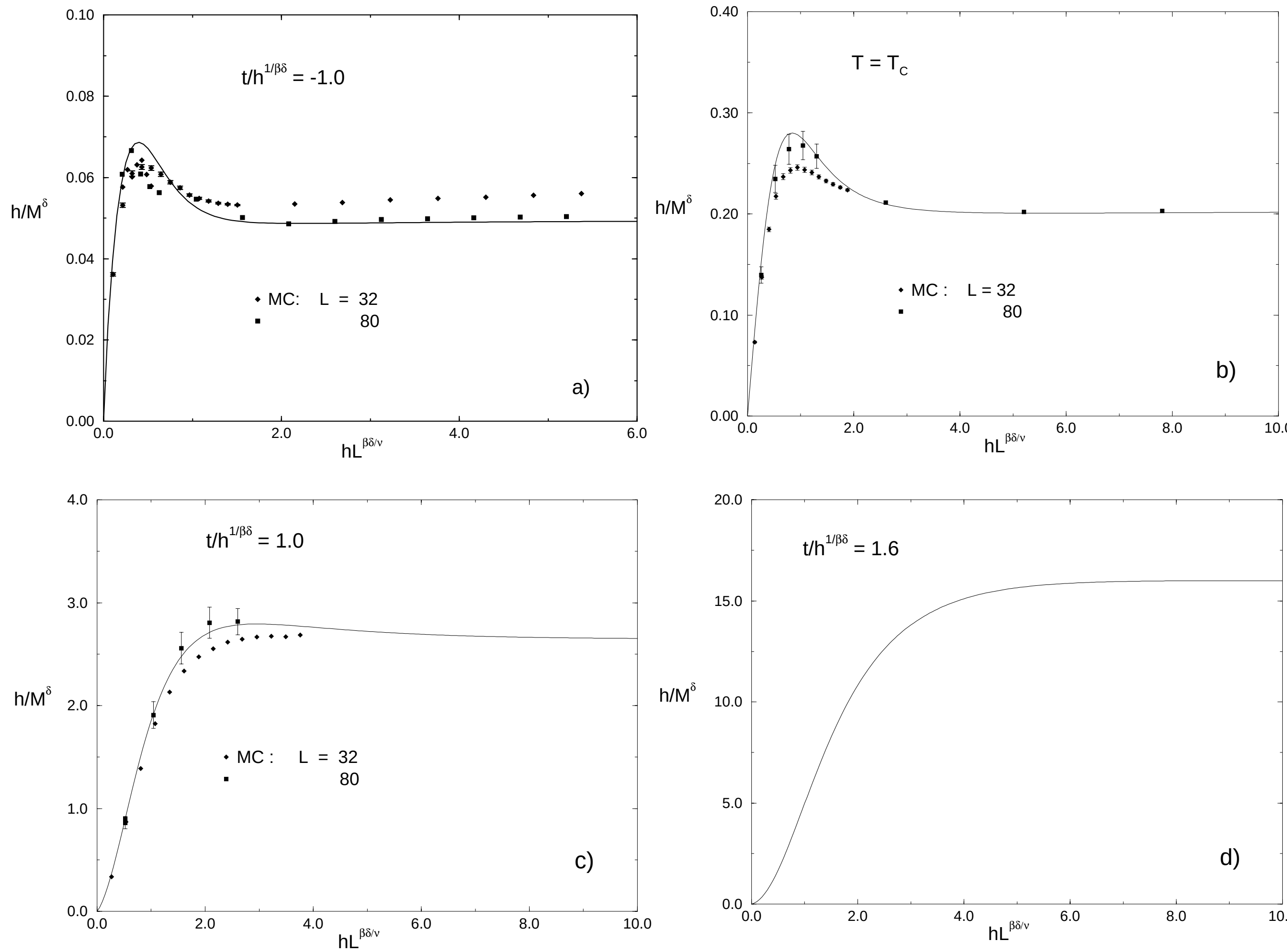

Fig. 1. Scaling plot (in units of the lattice constant, see Ref. [9]) of h/M^δ *versus* $x = hL^{\beta\delta/\nu}$ below T_c with (a) $t/h^{1/\beta\delta} = -1.0$, (b) $t/h^{1/\beta\delta} = 0$ (that means $T = T_\mathrm{c}$), (c) $t/h^{1/\beta\delta} = 1.0$, and (d) $t/h^{1/\beta\delta} = 1.6$. Monte Carlo data for $L = 32$ and 80. Solid line is the theoretical prediction equations (23-26); no Monte Carlo data are shown in part (d), where h/M^δ is a monotonic function of external field $x = hL^{\beta\delta/\nu}$.

4 Results and discussion

Figure 1 compares our Monte Carlo results for 32^3 and 80^3 spins with our theoretical predictions (Eqs. (23-26)), and shows good quantitative agreement; below T_c a pronounced peak is seen in the scaling function (Fig. 1a), at T_c it is somewhat weaker (Fig. 1b), above T_c it is barely visible (Fig. 1c), and far above T_c (Fig. 1d) it has vanished. The simulations, which at $T = T_\mathrm{c}$ have an accuracy of the order of one and five percent for $L = 32$ and 80, respectively, agree nicely with the theoretical predictions within the error bars of the MC data. (Far above T_c therefore no simulations were made.)

Thus, if one tries to determine the bulk critical amplitude of h/M^δ at the critical isotherm, then with varying L at a fixed field one first gets a too small value (left border of the figures), then a too high value (peak), and then a roughly correct value (plateau in the right part of the figure).

These non-monotonicities do *not* vanish if we take the lattices large enough. They are part of the asymptotic scaling function and thus whatever lattice size L we take there will be a field $h \propto 1/L^{\beta\delta/\nu}$ where h/M^δ has a maximum and near which it thus varies non-monotonically with L.

We also tested the prediction of [11,12] that for fixed $T < T_\mathrm{c}$ the leading finite-size deviation from the bulk value of M should vanish exponentially in L, and not with a power law $\propto 1/L^d$ (as predicted by perturbation theory based on the separation of the zero-mode [4–7,13]). Figure 2a shows again non-monotonic behaviour, in both three and five dimensions. But only in three dimensions these data are accurate enough to distinguish between a tail varying exponentially and one $\propto 1/L^d$; Figure 2b clearly supports the theoretically predicted [11,12] exponential variation. (These three-dimensional data were taken with Ito's fast algorithm [19].) Similarly, on the $d = 2$ square lattice at $T/T_\mathrm{c} = 0.99$, the exponential approach $\propto \exp(-L/18)$ towards the bulk magnetization fitted better than a L^{-2} power law, as shown in Figure 2c.

In order to make contact with $d = 3$ bulk properties we also used simulations at the critical isotherm with 1292^3

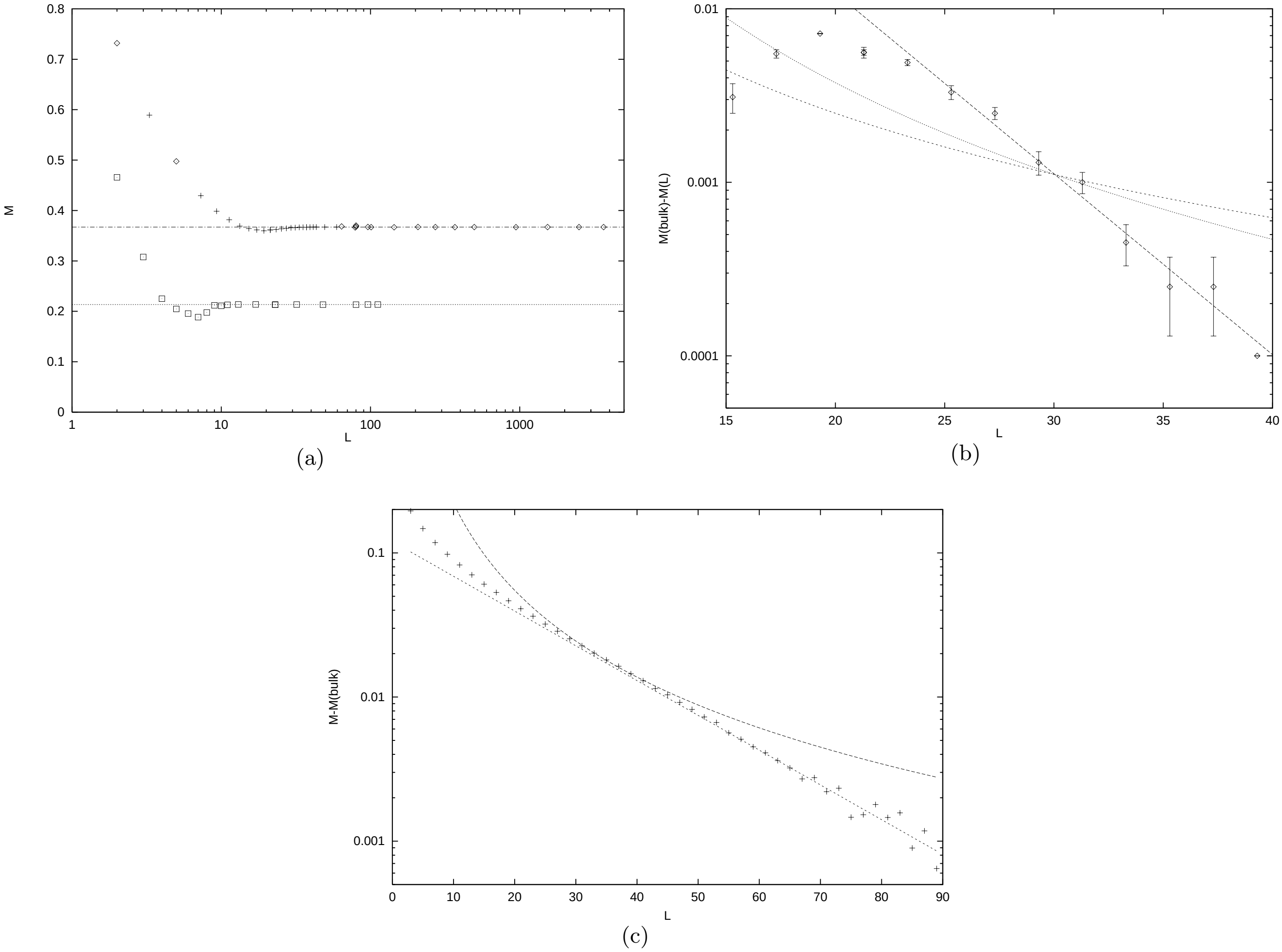

Fig. 2. (a) Monte Carlo data for the spontaneous magnetization in units of the lattice constant in three (diamonds and pluses) and five (square) dimensions at $T/T_{\mathrm{c}} = 0.99$, *versus* linear lattice size L. The horizontal line $M = 0.3671$ for three dimensions is determined from $L = 2496$. (b) Selected three-dimensional data from part (a) are shown as $M(L = \infty) - M(L)$ *versus* L in a semilogarithmic plot. The straight line represents an exponential decay [11,12], the two curved lines are power law decays $1/L^2$ and $1/L^3$ which fail to fit the data. The five-dimensional data of part (a) were not accurate enough to distinguish between an exponential and a $1/L^5$ decay. (c) Two-dimensional simulations (128 lattices for 10 million iterations each) in a semi-logarithmic representation at $T/T_{\mathrm{c}} = 0.99$. The straight line varies proportionally to $\exp(-L/18)$ and fits much better than the curve $\propto 1/L^2$.

spins [16]. From the simulations we obtain the bulk value of h/M^δ as $D_{\mathrm{c}} = 0.21 \pm 0.02$. Our field-theoretic result in equation (28) is in very good agreement with this value.

It is interesting to compare our simulation result also with other bulk theories. From series expansion Zinn and Fisher [18] obtained $C^{\mathrm{c}} = 0.299$ for the amplitude of the bulk susceptibility at the critical isotherm $\chi = C^{\mathrm{c}}|h|^{-\gamma/\beta\delta}$ with $\gamma = 1.2395, \nu = 0.6320$. This leads to $D_{\mathrm{c}} = 0.182$ according to the relation $D_{\mathrm{c}} = (C^{\mathrm{c}}\delta)^{-\delta}$.

D_{c} is also contained in the universal combination of amplitudes [17]

$$R_\chi = \Gamma D_{\mathrm{c}} A_M^{\delta-1} \tag{29}$$

where Γ is the amplitude of the bulk susceptibility $\chi = \Gamma t^{-\gamma}$ above T_{c} at $h = 0$ and A_M is the amplitude of the spontaneous magnetization $M_{\mathrm{bulk}} = A_M|t|^\beta$ below T_{c}. Using φ^4 field theory at $d = 3$ dimensions Guida and Zinn-Justin [1] have obtained $R_\chi = 1.649$. They also used the $\epsilon = 4 - d$ expansion and obtained $R_\chi = 1.674$ at $\epsilon = 1$. Using these values for R_χ and the high-temperature series expansion results [15] $\Gamma = 1.0928$, $A_M = 1.71$ and $\delta = (d\nu + \gamma)/(d\nu - \gamma)$ with $\gamma = 1.2395, \nu = 0.6335$, we obtain from equation (29) $D_{\mathrm{c}} = 0.205$ ($d = 3$ field theory) and $D_{\mathrm{c}} = 0.202$ (ϵ-expansion), respectively, in good agreement with our theoretical result, equation (28), and with our MC simulation.

In summary, our simulations confirmed *a posteriori* our theoretical predictions of Section 2 for the asymptotic finite-size effects in the three-dimensional Ising model. The agreement in Figure 1 is remarkable in view of the fact that the non-universal parameters of the theory were adjusted only to *bulk* parameters of the Ising model at $h = 0$ and not to any finite-size MC data.

Note added in proof

Improved simulations for five dimensions give for $7 \leq L \leq 13$ better agreement with an exponential size dependence than with one $\propto 1/L^5$.

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