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Critical Properties and Finite-Size Effects of the Five-Dimensional Ising Model

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Dedicated to Prof. Dr. H.E. Müser on the occasion of his 60th birthday

Monte Carlo calculations of the thermodynamic properties (energy, specific heat, magnetization suceptibility, renormalized coupling) of the nearest-neighbour Ising ferromagnet on a five-dimensional hypercubic lattice are presented and analyzed. Lattices of linear dimensions $L=3$, 4, 5, 6, 7 with periodic boundary conditions are studied, and a finite size scaling analysis is performed, further confirming the recent suggestion that L does not scale with the correlation length ξ (the temperature variation of which near the critical temperature T_c is $\xi \propto |1-T/T_c|^{-1/2}$), but rather with a "thermodynamic length" l (with $l \propto |1-T/T_c|^{-2/d}$, $d=5$ here). The susceptibility (extrapolated to the thermodynamic limit) agrees quantitatively with high temperature series extrapolations of Guttmann. The problem of fluctuation corrections to the leading (Landau-like) critical behaviour is briefly discussed, and evidence given for a specific-heat singularity of the form $|1-T/T_c|^{1/2}$, superimposed on its leading jump.

I. Introduction

One of the key insights of the modern theory of critical phenomena (see e.g. [1]) is the existence of a marginal dimensionality d^*: nontrivial critical exponents α, β, γ, ν, ... (of the specific heat C, order parameter m, susceptibility χ, correlation length ξ,...) occur only for system dimensionality $d<d^*$, due to strong fluctuation influence, wile for $d>d^*$ they have the values predicted from simple Landau theory [2]. While there fluctuation effects, which are neglected in Landau theory, thus do not affect the critical exponents of the leading singularities near the critical temperature T_c, they still are expected to govern the next-to-leading singular terms, and thus yield important corrections to scaling [3-5].
For Ising systems, $d^*=4$ and thus situations with $d>d^*$ are clearly not relevant experimentally. But checking the question whether one understands the systems with $d>d^*$ theoretically has some bearing on the theory of critical phenomena in general. For example, for $d>d^*$ the hyperscaling relation $d\nu=2-\alpha$ is no longer valid. Since the possibility has been raised that there might be a slight violation of this hyperscaling relation even for $d=3$ [6, 7], it is interesting to study systems with $d>d^*$ when this violation definitively occurs, as a testing ground. A particular interesting consequence of the failure of hyperscaling is the fact that also finite size scaling in its standard form [8, 9] then does not hold [10-14, 6]: the question then must be asked whether there is then a modified form of finite size scaling [11, 12, 14].
Apart from their theoretical interest, these questions may also be interesting experimentally for other systems where the marginal dimensionality d^* is lower. For uniaxial ferroelectrics and dipolar magnets, $d^*=3$ and the leading critical behaviour is identical to that of a four-dimensional short-range Ising system [15-17]; for certain second-order elastic structural transitions one indeed may have $d^*=2.5$ [18] and thus the case $d>d^*$ may be physically realized [18, 19]. Other problems where d may exceed d^* are certain kinetic models, such as the so-called "true self-avoiding walk" which has $d^*=2$ [20]. Finally, a situation with a large value of d^* ($d^*=6$) but a

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violation of hyperscaling is likely to occur in systems with quenched random fields: various arguments predict that the universal critical properties of the impure system in d dimensions are identical to those of the corresponding pure system in d' dimensions, with either [21] $d'=d-2$ or [22] $d'=d-2+\eta(d')$, η being the critical exponent describing the decay of the correlation function at criticality. If such a shift of effective dimensionality occurs, the hyperscaling relation could be modified to $d'\nu=2-\alpha$.

The present work is devoted to a study of the five-dimensional nearest-neighbour Ising model. The aim of this work is to show that the numerical data are indeed nicely consistent with the critical behaviour expected on the general theoretical grounds mentioned above. So evidence for both the Landau behaviour of the leading terms and a non-Landau behaviour of the subleading terms (such as an anomaly $\Delta C \propto |1-T/T_c|^{1/2}$ in the specific heat) will be presented. Particular attention will be paid to an analysis of finite size effects, since the nature of finite size scaling for $d>d^*$ has been a subject of extensive, and sometimes controversial, discussions [11, 12, 14, 23]. In fact, preliminary results of the present investigation where the so-called renormalized coupling constant was analyzed [14] have contributed to settle this issue. The present paper thus tries to elucidate more completely how to do finite size scaling above four dimensions.

In Sect. II we shall describe the "raw data" of this Monte Carlo investigation while Sect. III will present a discussion of critical properties. Sect. IV then presents a detailed finite size scaling analysis, and Sect. V summarizes our conclusions.

II. Monte Carlo Results for the Thermal Properties of Finite Five-Dimensional Ising Lattices

Standard Monte Carlo calculations [24] have been performed for the Ising Hamiltonian in zero magnetic field and exchange interaction J,

$$\mathscr{H}=-J\sum_{\langle i,j\rangle} S_i S_j, \qquad S_i=\pm 1 \tag{1}$$

where i labels the sites of a hypercubic five-dimensional lattice with linear dimensions $L=3, 4, 5, 6, 7$ and periodic boundary conditions in all lattice directions. The symbol $\langle i,j\rangle$ indicates that the sum runs over nearest-neighbour pairs once. Typically, for each size about 15–30 temperatures k_BT/J in the vicinity of the bulk critical temperature ($\tanh(J/k_BT_c)=0.113427\pm0.000007$ [5], i.e. $k_BT_c/J\approx 8.77$) were studied. While for the smaller systems the equilibration time was chosen 6000 Monte Carlo steps (MCS) per spin and the subsequent 10000 MCS/spin were kept for data analysis, close to T_c as well as for the larger systems all times were chosen 3–4 times as large, and in a few cases runs were repeated with other random numbers and averaged together, in order to obtain appropriate statistical accuracy. This statistical effort (rather than any storage limitations) prevented us to go to systems larger than $N_{\max}=7^5=16807$. Previous work (except Ref. 14) on this model was restricted to one size ($L=6$) only and nothing but the magnetization was presented [25]; as will become clear from our analysis this previous study could not significantly address the questions about the critical behaviour of the model (moreover, the critical temperature $k_BT_c/J=8.70$ chosen in Ref. 25 is nearly one percent too low).

Quantities calculated in our study include the absolute value of the magnetization ($N=L^5$)

$$\langle |S|\rangle_L=\frac{1}{N}\langle|\sum_i S_i|\rangle, \tag{2}$$

the mean square magnetization

$$\langle S^2\rangle=\frac{1}{N^2}\langle(\sum_i S_i)^2\rangle \tag{3}$$

the fourth moment of the magnetization distribution

$$\langle S^4\rangle_L=\frac{1}{N^4}\langle(\sum_i S_i)^4\rangle, \tag{4}$$

the internal energy per spin $U=\langle\mathscr{H}\rangle/N$ and the specific heat per spin calculated from energy fluctuations

$$C/k_B=(\langle\mathscr{H}^2\rangle-\langle\mathscr{H}\rangle^2)/(N[k_BT]^2). \tag{5}$$

Also the susceptibility per spin is obtained from Eqs. (2), (3) via a fluctuation relation

$$\chi=N(\langle S^2\rangle_L-\langle|S|\rangle_L^2)/(k_BT); \tag{6a}$$

while this relation is particularly useful for $T<T_c$, one may use for $T>T_c$ the alternative relation

$$\chi'=N\langle S^2\rangle_L/(k_BT). \tag{6b}$$

Of course, the quantities C, χ, χ' defined above also will have an explicit size-dependence. Finally, Eqs. (3), (4) allow to compute the so-called renormalized coupling constant g_L [12–14]

$$g_L=-3+\langle S^4\rangle_L/\langle S^2\rangle_L^2. \tag{7}$$

The numerical results for these quantities are presented in Figs. 1–6. The estimate for the critical tem-

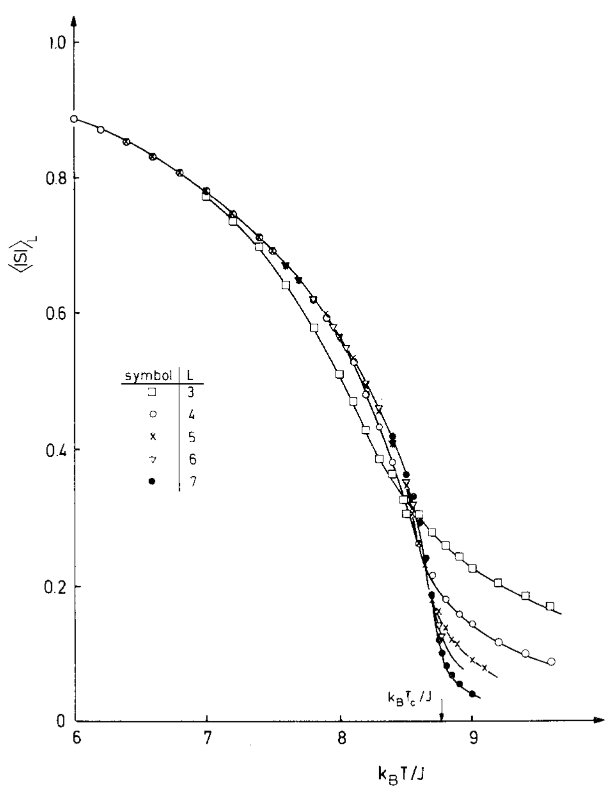

Fig. 1. Magnetization $\langle |S| \rangle_L$ of finite five-dimensional Ising systems plotted versus temperature. Various linear dimensions are shown by different symbols as indicated. Arrow shows the critical temperature found from extrapolation of the high temperature series expansions [5, 26]. Curves are only drawn to guide the eye

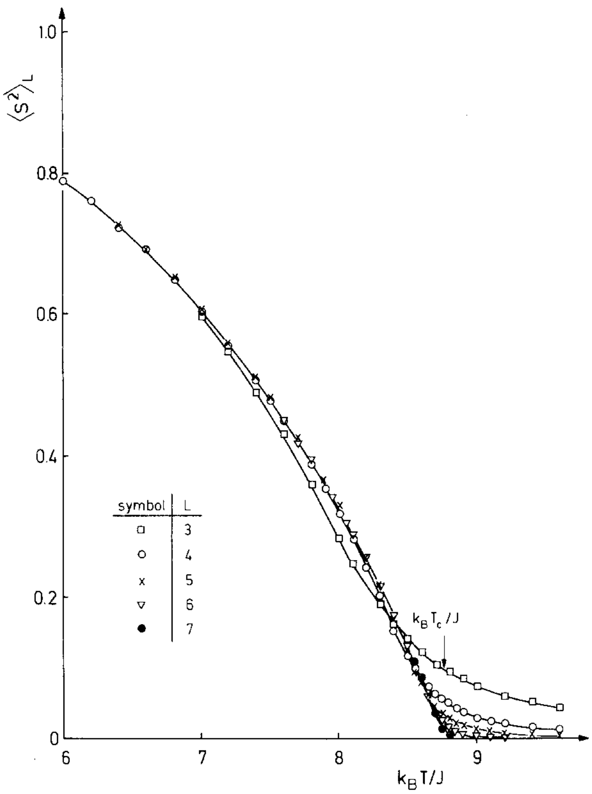

Fig. 2. Mean square magnetization $\langle S^2 \rangle_L$ plotted vs. temperature. For further explanations see Fig. 1

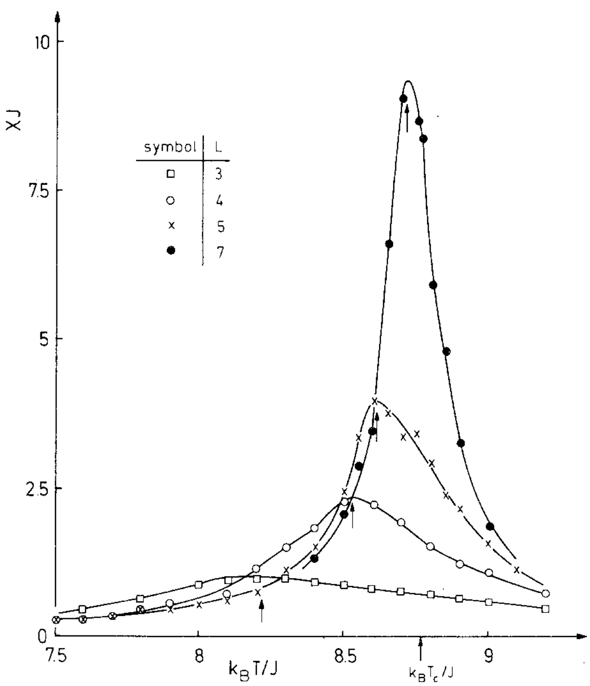

Fig. 3. Susceptibility per spin χ plotted vs. temperature. Arrows indicate the position of the susceptibility maximum

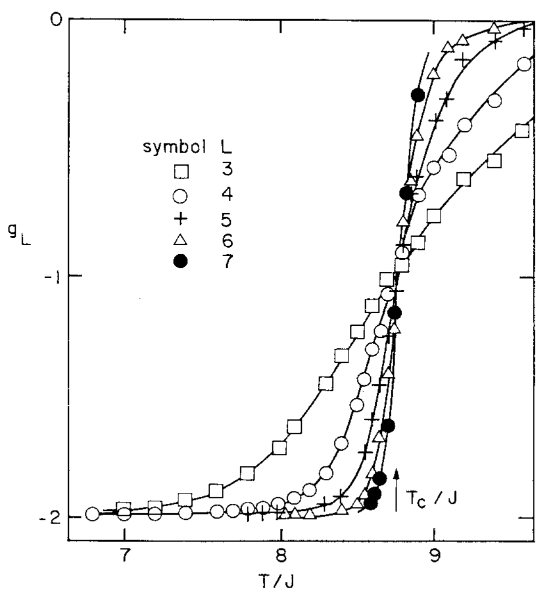

Fig. 4. Renormalized coupling constant g_L plotted vs. temperature

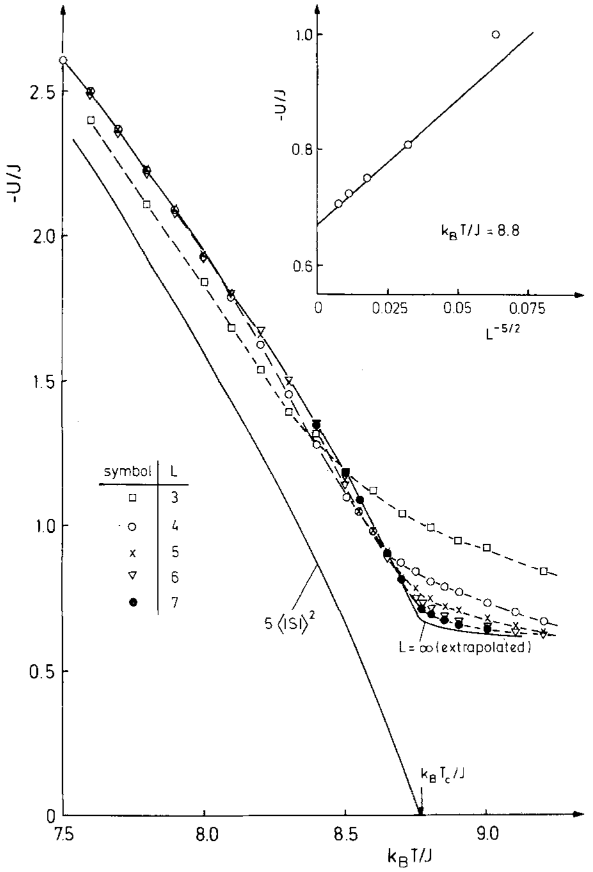

Fig. 5. Internal energy per spin plotted vs. temperature. At $T \gtrsim T_c$ also the energy extrapolated to the thermodynamic limit, $L=\infty$, is included. The insert shows how this extrapolation is performed, choosing as an example the temperature $k_B T/J = 8.8$. Using the data of Fig. 1, the "order-parameter-contribution" to the energy $5 \langle |S| \rangle^2$ is shown for comparison

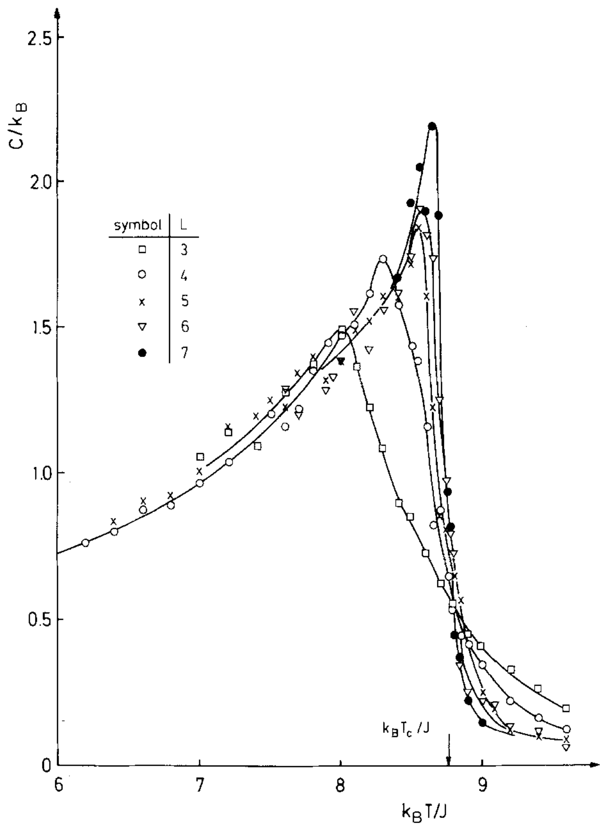

Fig. 6. Specific heat per spin plotted vs. temperature

perature shown, is that of the high temperature series expansions [5, 26]. The curves for $\langle |S| \rangle_L$ and $\langle S^2 \rangle_L$ show the "finite-size-tails" above T_c as usual. Both the peaks of the susceptibility and of the specific heat are shifted towards lower temperature with decreasing system sizes. From all these data on the magnetization, susceptibility and specific heat it would be difficult to accurately estimate the bulk critical temperature directly, as it also happens for lower-dimensional systems [13]. Again one finds that the "renormalized coupling" g_L is most useful for finding directly the critical temperature (as in the lower dimensional case [13]). The behaviour of g_L for both low and high temperatures is trivial [13]: For $L\to\infty$ and $T<T_c$ we must have $\langle S^2 \rangle_L \to m^2$, where m is the spontaneous magnetization, and similarly $\langle S^4 \rangle_L \to m^4$: hence $\langle S^4 \rangle_L \approx \langle S^2 \rangle_L^2$ and thus $g_L = -2$. In the paramagnetic regime, on the other hand, the magnetization distribution is Gaussian and hence $\langle S^4 \rangle_L \to 3 \langle S^2 \rangle_L^2$ for $L\to\infty$, and hence $g_L \to 0$ for $T>T_c$. Thus a nontrivial behaviour of g_L is found for each L only for this temperature regime over which the transition from the disordered to the ordered state is smeared out. As a consequence, it was pointed out in Ref. 13 that one can find an estimate $T_c(L,L')$ for the bulk value of T_c from the intersection of two curves g_L and $g_{L'}$; since the temperature width over which this rounding occurs must shrink to zero as L or L' tend to infinity we must have $\lim_{L\to\infty} T_c(L,L') = T_c$, for any fixed L'. What is seen in Fig. 4 is that within the desired accuracy of $\Delta T/T_c \approx 10^{-3}$ all curves g_L actually intersect in the same point, and hence yield an estimate for T_c even without any extrapolation to $L\to\infty$, to that accuracy. It is gratifying that this estimate, $k_B T_c/J \approx 8.77$, precisely coincides with the result of the high temperature series extrapolation mentioned above [5, 26].

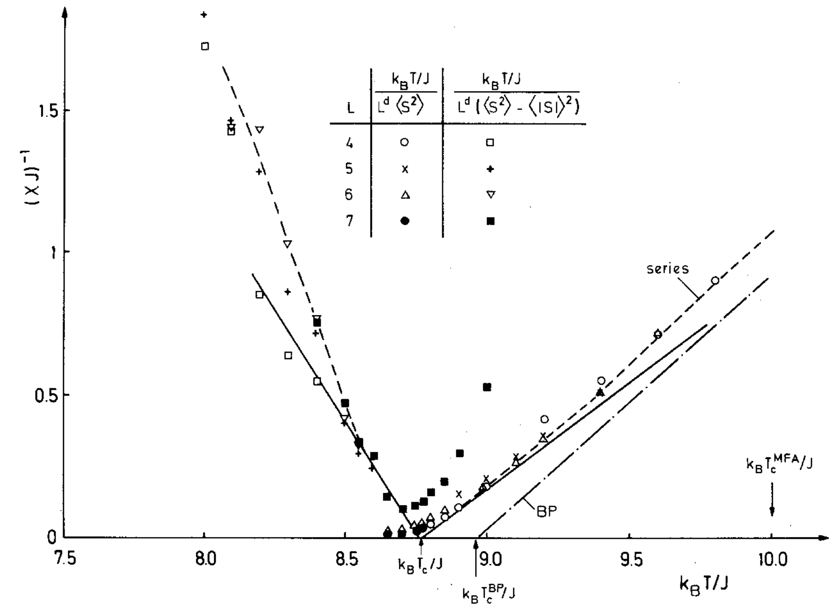

Fig. 7. Inverse susceptibility plotted vs. temperature. Both data for χ [Eq. (6a) and χ' Eq. (6b)] are shown. Dash-dotted line indicates the behaviour predicted by the Bethe-Peierls-approximation [Eqs. (9), (10) with $k_B T_c^{BJ}/J \approx 8.96$] [27]. Also the molecular field-estimate of the critical temperature is shown. The broken curve for $T > T_c$ is due to the series expansion [5], Eq. (11), while the analoguous broken curve for $T < T_c$ is freely drawn through the points to guide the eye. Full straight lines are expected asymptotic laws (Eqs. (9)) with the high temperature series estimates for T_c and Γ_+ (using $\Gamma_- = \Gamma_+/2$)

While in lower dimensionality the internal energy often exhibits relatively little size-dependence, in the present case the size-dependence is rather pronounced. Thus it was necessary to perform an extrapolation to the thermodynamic limit in the temperature regime $0.99\,T_c \lesssim T \lesssim 1.1\,T_c$; as indicated this extrapolation was performed graphically by plotting the energy $vs \cdot L^{-5/2}$. The choice of this particular exponent is dictated by the finite size scaling considerations described in Sect. IV. As expected, the variation of U with this variable is found to be linear. It is seen that one finds a kink-like singularity of the energy at T_c. This behaviour, of course, again is not unexpected: if molecular-field theory were valid, the internal energy would be simple expressed in terms of the magnetization as $U = -5Jm^2$ (for a nearest-neighbour Ising model in five dimensions). Thus a curve displaying this part of the energy simply induced by the order parameter is included in Fig. 5. The total internal energy includes also a fluctuation part, not included by the molecular field approximation, which has a rather smooth temperature variation throughout the critical region. This fluctuation contribution is responsible for the nonzero internal energy at and above T_c. We estimate the internal energy at criticality as

$$U_c/J = -0.67 \pm 0.01. \tag{8}$$

This fluctuation contribution also is responsible for the fact that the specific heat maximum is considerably enhanced in comparison with the value which would be predicted by the molecular field approximation, which would be $C_{max}/k_B = 3/2$, see Fig. 6.

III. Critical Behaviour

We now turn to an analysis of the critical properties of the system. Since one expects Landau theory to be valid, the bulk susceptibility χ_b should behave for $L \to \infty$ approximately close to T_c as follows

$$\begin{aligned} k_B T\chi_b &\approx \Gamma_+(1 - T_c/T)^{-1}, \quad T \to T_c^+; \\ k_B T\chi_b &\approx \Gamma_-(1 - T_c/T)^{-1}, \quad T \to T_c^- \end{aligned} \tag{9}$$

with $\Gamma_- = \Gamma_+/2$ (also for amplitude ratios such as Γ_-/Γ_+ the Landau predictions should be valid). The behaviour of (9) suggests to plot the inverse susceptibility vs. temperature and this is done in Fig. 7. We have also included the critical temperature predicted by the molecular field approximation ($k_B T_c^{MFA}/J = 2d = 10$) and the Bethe-Peierls-approximation [27] $\{k_B T_c^{BP}/J = 2/\ln(2d/(2d-2)) \approx 8.96\}$, which both are significently off. While in the molecular field approximation the amplitude Γ_+ in Eq. (9) simply is $\Gamma_+ = 1$, in the Bethe-Peierls approximation we have [27, 28]

$$\Gamma_+ = \frac{2}{d-2} \Big/ \ln\left(\frac{2d}{2d-2}\right) \approx 1.12. \tag{10}$$

The high temperature series analysis [5] reveals that the amplitude Γ_+ is even more enhanced, $\Gamma_+ \approx 1.295$, and there is also a singular correction term $\{v \equiv \tanh(J/k_B T)\}$

$$k_B T\chi_b = 1.311(1 - v/v_c)^{-1} - 0.48(1 - v/v_c)^{-1/2}, \quad v \lesssim v_c \tag{11}$$

Equation (11) is included in Fig. 7 and it is seen to be reasonably consistent with the Monte Carlo data for χ' Eq. (6b); above T_c the Monte Carlo data for χ [Eq. (6a)] are still far from the asymptotic regime where χ becomes independent of size, and hence can not be used to infer anything about the critical behaviour directly. Very close to T_c also the data for χ' start to deviate from (11) but at the same time start to become distinctly size-dependent, and hence this deviation is clearly a finite size effect. It is also seen that the leading term in (11) alone would describe χ accurately, within our statistical errors, only up to temperatures about $k_B T/J \approx 9.0$, i.e. for $|1-T/T_c| \lesssim 0.025$, while outside of that temperature region the singular correction term already becomes numerically important. A similar correction seems to exist below T_c, where the data for χ (in the regime $k_B T/J \lesssim 8.5$ where the size-dependence for $L \gtrsim 6$ is smaller than the statistical error) fall above the asymptotic straight line in Fig. 7. Of course, data for much larger sizes and better statistical accuracy would be required to actually show more convincingly that the leading correction to the Landau behaviour, Eq. (9), has the singular form shown in (11).

A more convincing evidence for singular corrections comes from an examination of the specific heat data, Fig. 6, where for $d>4$ one expects a behaviour of the form [5]

$$C = C_{\max} - \text{const}\,|1-T/T_c|^{(d-4)/2}, \qquad T \to T_c^-, \tag{12}$$

and a similar behaviour (with a different leading term) above T_c. For $d=5$ Eq. (12) would imply a square root-like anomaly, and this is in fact consistent with the data. Unfortunately, it is not possible to estimate the leading term $C_{\max}$ with high accuracy (Fig. 8); trying various extrapolations we only can say that

$$C_{\max}/k_B = 2.3 \pm 0.3. \tag{13}$$

However, using this estimate in Fig. 6 to obtain the subleading contribution $\Delta C = C_{\max} - C$ we find that the data for ΔC are indeed consistent with a variation $\Delta C \propto (1-T/T_c)^{1/2}$ over a wide temperature regime (Fig. 9). Since the data for ΔC shown in this log-log plot are not so close to T_c, this conclusion is not so much affected by the uncertainty in the precise value of $C_{\max}$.

Finally, we turn to the critical behaviour of the magnetization, which also is displayed in Fig. 9. In principle, both $\langle S^2 \rangle_L$ and $\langle |S| \rangle_L^2$ are equally well suited for an extrapolation towards $L \to \infty$, but Fig. 9

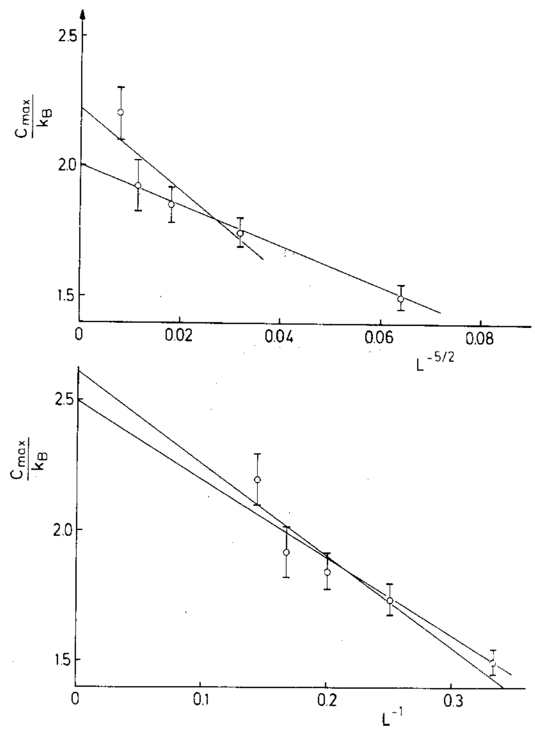

Fig. 8. Maximum value of the specific heat $C_{\max}$ plotted vs. $L^{-5/2}$ (upper part) and plotted vs. L^{-1} (lower part). Straight lines indicate various possible extrapolations

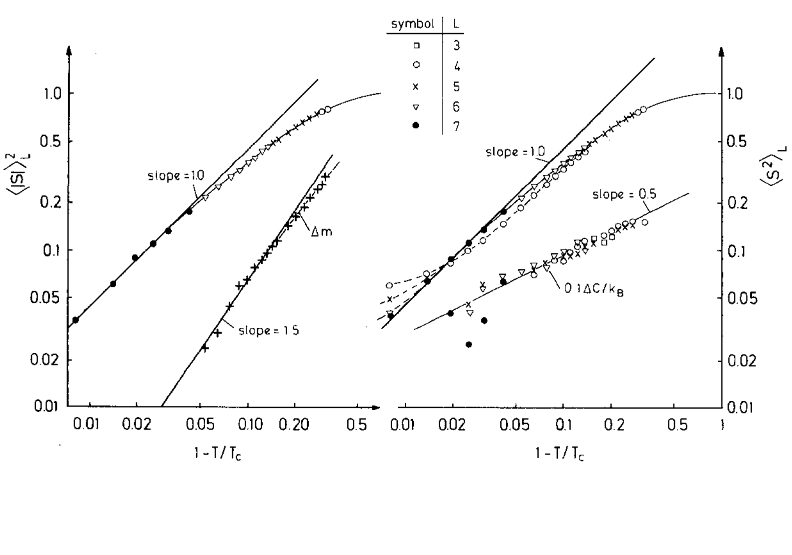

Fig. 9. Log-log plot of the magnetization square $\langle |S| \rangle_L^2$ (left part) and $\langle S^2 \rangle_L$ (right part) vs. $1-T/T_c$. The estimated asymptotic critical behaviour of both quantities for $L=\infty$ is indicated by the straight line with slope unity. The deviation Δm between the asymptotic law and the actual magnetization is shown on the left, the specific heat difference $\Delta C = C_{\max} - C$ is shown on the right

shows that the finite size effects for $\langle|S|\rangle_L^2$ are somewhat smaller than those for $\langle S^2\rangle_L$, and hence the convergence to the thermodynamic limit is somewhat more rapid for $\langle|S|\rangle_L^2$ than for $\langle S^2\rangle_L$. But both sets of data seem to be consistent with a behaviour of the bulk spontaneous magnetization m_b

$$m_b^2 = B^2(1-T/T_c), \quad T\to T_c, \quad B^2 \approx 4.4 \pm 0.2. \tag{14}$$

In molecular field theory, $B^2=3$ and hence we again find that the actual amplitude is somewhat enhanced [29].

From Fig. 9 it is seen that the deviations from (14) occur for $(1-T/T_c)\gtrsim 0.04$. In order to analyze these deviations we also plot the quantity $\Delta m = |\langle|S|\rangle_L - B(1-T/T_c)^{1/2}|$. The data seem to imply $\Delta m \propto (1-T/T_c)^{3/2}$, which means that the correction terms are regular

$$m_b = B(1-T/T_c)^{1/2}\{1+B'(1-T/T_c)+\ldots\}. \tag{15}$$

Of course, it is possible that there exists a singular correction (Δm proportional to $(1-T/T_c)^1$ yielding a term $B''(1-T/T_c)^{1/2}$ in Eq. (15)) for the magnetization as well as it seems to exist for susceptibility (Eq. (11)) and specific heat (Eq. (12)), but then its amplitude B'' is probably much smaller than the amplitude B'. While the available data are not for large enough sizes to probe the region extremely close to T_c, which would be necessary to convincingly clarify the nature of these correction terms, they do show that pronounced correction effects to the leading Landau-like critical behaviour do exist in this five-dimensional Ising model.

IV. Finite Size Scaling

In Ref. 14 it was suggested that the free energy density for $d>d^*$ satisfies a scaling hypothesis where a dangerous irrelevant variable [30, 11] u must be taken into account:

$$f_L = L^{-d} f(tL^{y_T}, hL^{y_H}, uL^{y_u}) \tag{16}$$

where $t=T/T_c-1$, h is the magnetic field, and y_T, y_H, y_u are renormalization group exponents ($y_T=1/\nu$, $y_H=(\gamma+\beta)/\nu$). The variable u is irrelevant, $y_u<0$, but dangerous since $f(x,y,z)$ is singular for $z\to 0$, i.e. in this limit Eq. (16) is replaced by

$$f_L = L^{-\tilde{d}^*}\tilde{f}(tL^{y_T^*}, hL^{y_H^*}), \tag{17}$$

where $\tilde{d}^*$, y_T^*, and y_H^* are a new set of exponents, and where consistency with the bulk critical behaviour in the thermodynamic limit requires

$$y_T^* = \frac{\tilde{d}^*}{\gamma+2\beta}, \quad y_H^* = \frac{\tilde{d}^*(\gamma+\beta)}{\gamma+2\beta}. \tag{18}$$

Since the renormalized coupling constant g_L can be written as [14]

$$g_L = (\partial^4 f_L/\partial h^4)/[L^d(\partial^2 f_L/\partial h^2)^2]|_{h=0}. \tag{19}$$

Equation (17) also implies [14]

$$g_L = L^{\tilde{d}^*-d}\tilde{g}(tL^{y_T^*}). \tag{20}$$

The value of $\tilde{d}^*$ and hence of y_T^* (Eq. (18)) has been controversal [12, 14, 23]. In Ref. 14 the relation $\tilde{d}^* = d$ was derived, however, which in turn implies

$$y_T^* = d/(\gamma+2\beta). \tag{21}$$

Since Eq. (17) can be interpreted as saying that L scales with a length l,

$$l \propto t^{-1/y_T^*} = t^{-(\gamma+2\beta)/d} \tag{22}$$

we conclude the following: if the hyperscaling relation $d\nu=\gamma+2\beta$ is valid, the length l defined in (22) would simply be proportional to the correlation length ξ (and hence not be an independent new length at all). Conversely, if hyperscaling is invalid, the exponent $1/y_T^*$ differs from ν, and the thermodynamic length l has a temperature dependence different from the correlation length. Note that for $d>d^*$, where this happens, the divergence of l is weaker than the divergence of ξ. Under these circumstances, the statement embodied in (16)-(22), that L scales with the thermodynamic length l rather than with ξ, may look surprising. Thus we also quote a somewhat less formal argument [14] to support (21): the probability distribution of the magnetization s in a finite cube of linear dimension L for $T<T_c$ and L large enough tends to *a* sum of two Gaussians, centered around the bulk spontaneous magnetization $\pm m_b$,

$$P_L(s) = \frac{L^{d/2}}{2\sqrt{2\pi k_B T\chi_b}}\{e^{-(s-m_b)^2L^d/2k_BT\chi_b} + e^{-(s+m_b)^2L^d/2k_BT\chi_b}\}. \tag{23}$$

In Eq. (23), thermodynamic fluctuation theory [2] links the widths of these distributions to the bulk susceptibility χ_b. Hence the arguments of the experimental functions can be cast into the form

$$\frac{(s|t|^{-\beta}\mp B)^2}{2\Gamma^-}|t|^{2\gamma+\beta}L^d = \frac{(s|t|^{-\beta}\mp B)^2}{2\Gamma}(L/l)^d \tag{24}$$

where l is given by (22). Hence Eq. (23) requires indeed that the variable $tL^{y_T^*}$ must appear in the free energy f_L and its derivatives (which also can be constructed as moments of the distribution $P_L(s)$), at least for $L\to\infty$. The assumption equivalent to (16) then is that the variable L/l is the only combination in which the variables t, L enter. This assumption, of course, is nontrivial, and probably it is only true for periodic boundary conditions. In the case of free boundary conditions, there must be surface corrections f_s to the bulk free energy f_b, i.e.

$$f_L \xrightarrow[L\to\infty]{} f_b(t,h)+L^{-1}f_s(t,h). \tag{25}$$

But Eq. (17) implies, if there were a correction proportional to L^{-1}

$$f_L \xrightarrow[L\to\infty]{} t^{\gamma+2\beta}\tilde{f}_b\{t^{-(\gamma+\beta)}h\} + L^{-1}\,t^{(\gamma+2\beta-1/y_T^*)}\tilde{f}_S\{t^{-(\gamma+\beta)}h\}. \tag{26}$$

As a consequence the surface free energy would vanish at T_c with a critical exponent $2-\alpha_s=(\gamma+2\beta-1/y_T^*)$. However, the Landau theory for semiinfinite geometry shows that the surface free energy vanishes with an exponent $2-\alpha_s=(\gamma+2\beta-\nu)$ [31]. Therefore, we conclude that (16)–(24) are not applicable for $d>d^*$ in the case of free surfaces [14].

In the following we analyze our Monte Carlo data in the light of this scaling analysis (extending Ref. 14 where the data on the renormalized coupling constant were already presented and analyzed). A key consequence of (17)–(22) is that any possible definitions for a shift of the effective critical temperature $T_c(L)$ of the finite system lead to

$$T_c(L)-T_c=\Delta T_c \propto L^{-y_T^*}=L^{-5/2} \quad (d=5). \tag{27}$$

In Fig. 10 this behaviour is verified both for the susceptibility χ and the specific heat, defining $T_c(L)$ from the temperature where the maxima of these quantities occur. Note that these maxima do not

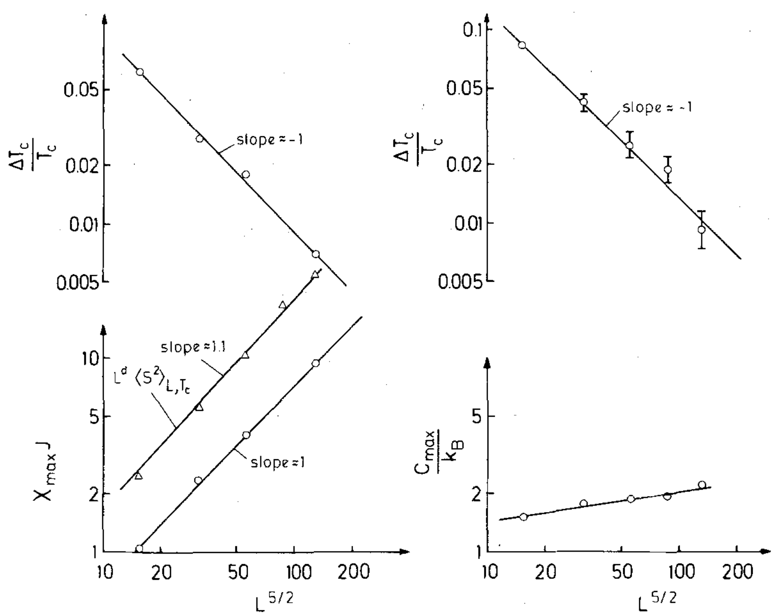

Fig. 10. Log-log plot of the relative shift of the critical temperature vs. $L^{5/2}$ for the susceptibility (upper left part) and specific heat (upper right part), and of the maximum susceptibility χ_{max} (lower left part) and specific heat (lower right part). Also the value of χ' at the bulk T_c is included (Eq. (6b), lower left part of this figure). Straight lines indicate the respective power laws

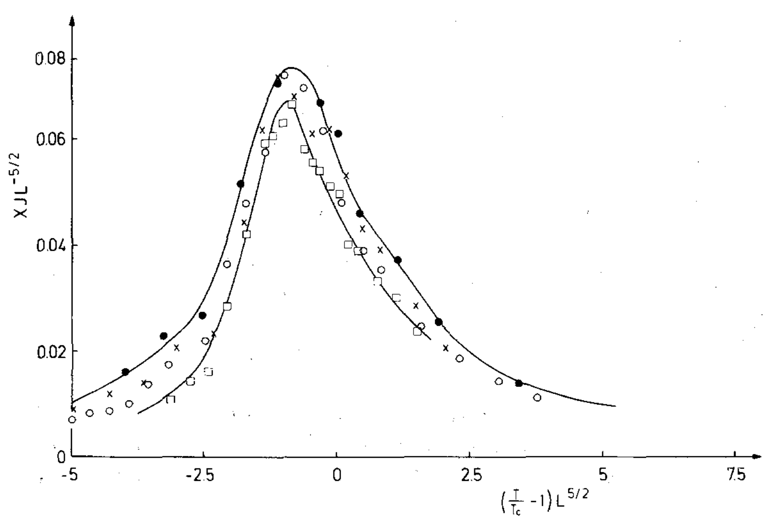

Fig. 11. Scaling plot of the susceptibility, $\chi J L^{-5/2}$ is being plotted vs. $(T/T_c-1)L^{5/2}$, for various values of L (symbols have same meaning as in Fig. 3). Curves are drawn through the data for $L=3$ and $L=7$ to guide the eye

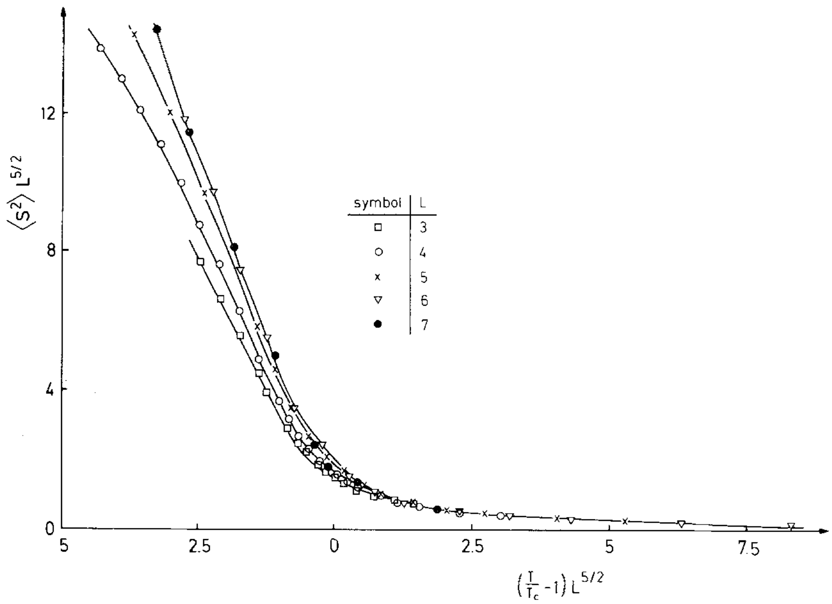

Fig. 12. Scaling plot of the magnetization square $\langle S^2\rangle L^{5/2}$ vs. $(T/T_c-1)L^{5/2}$, for various values of L. Curves are only drawn to guide the eye

occur at the same temperatures, indicating the fact that there is no uniquely defined $T_c(L)$, as expected. The analysis of the height of these maxima is somewhat less convincing: while $\chi_{\max} \propto L^{5/2}$ with very good accuracy, $L^d\langle S^2\rangle_{L,T_c}$ seems to indicate an exponent 10% too high, and the same is true for $C_{\max}$ (actually we expect that $C_{\max}(L\to\infty)$ tends to a finite constant, see Fig. 8 and Eqs. (12), (13)).

Of course, not only should the peak position and height of χ scale with the expected power laws, but Eq. (17) also implies, for $\gamma=1$,

$$\chi L^{y_T^*} = \tilde{\chi}(t L^{y_T^*}) \tag{28}$$

where $y_T^* = 5/2$ in $d=5$. Equation (28) is checked in Fig. 11, using the bulk value of T_c due to the series expansion [5], i.e., there are no adjustable parameters. While the data for $L=3,4$ seem to fall off the scaling function, the data for $L=5,7$ already seem to scale rather well. Of course, since correction terms to the relations (16)–(22) are expected, it is no surprise that in Fig. 11 systematic deviations from a collapse of the data on a simple curve must occur. The same story is told by the data for $\langle S^2\rangle$, Fig. 12: While the data for $L=3,4$ are distinctly off the asymptotic curve for $T<T_c$, the data for $L=5$ are only slightly off, and the data for $L=6,7$ yield an identical curve. For $(T/T_c-1)L^{5/2} \lesssim -1$, this curve is essentially the straight line, Eq. (14), giving further credence to the estimated amplitude factor B there.

The most convincing evidence for the predicted finite size scaling behaviour comes from a study of g_L (which was presented earlier already in Ref. 14). As is evident from Fig. 13, basically all sizes from $L=3$ up to $L=7$ coincide on the same scaling function. The fact that $g_L = -3 + \langle S^4\rangle_L / \langle S^2\rangle_L^2$ scales better than $\langle S^2\rangle_L$ or $\langle S^2\rangle_L - \langle |S|\rangle_L^2$ do is probably due to a fortunate (at least approximate) cancellation of corrections to finite size scaling when one takes this ratio.

In Ref. 14 it was pointed out that one can in fact explain Fig. 13 in the spirit of Eq. (23): writing for $P_L(s)$ a Landau-like form

$$P_L(s) \propto \exp[-L^d(c t_L s^2 + u s^4)], \quad t_L = t - A L^{-d/2}, \tag{29}$$

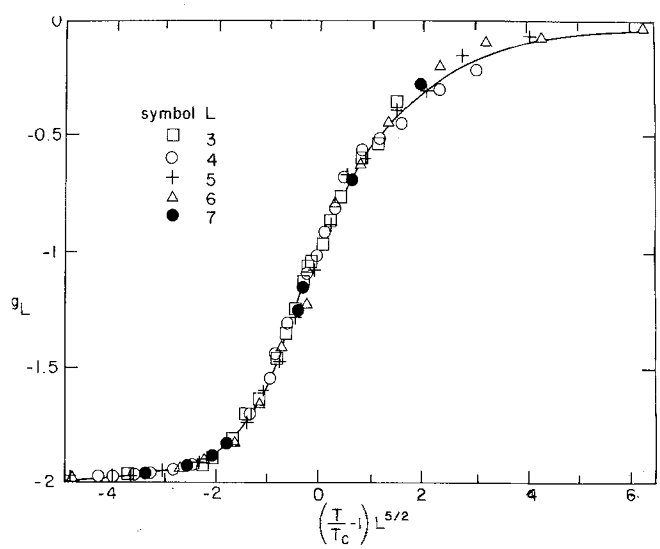

Fig. 13. The data for g_L shown Fig. 4 plotted vs. the scaling variable $(T/T_c-1)L^{5/2}$, for various values of L. The solid line is obtained from (31)

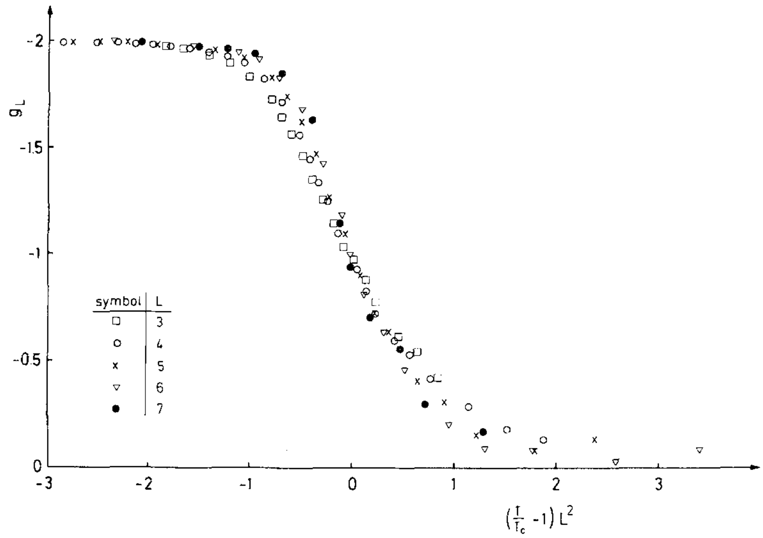

Fig. 14. Scaling plot of the renormalized coupling constant g_L using the (wrong) scaling variable $(T/T_c-1)L^{1/\nu}=(T/T_c-1)L^2$ of standard finite size scaling

where c, A and u are constants and rescaling s according to the substitution

$$\Phi=(uL^d)^{1/4}s \tag{30}$$

one finds

$$P_L(\Phi)\propto\exp[-a(L^{d/2}t-b)\Phi^2-\Phi^4], \tag{31}$$

where $a=c/u^{1/2}$, $ab=A$. The solid curve is obtained from calculating the second and fourth moment of Eq. (31), choosing $b=0.37$, $a=0.56$ [14]. It evidently fits the data well [32].

Finally, Fig. 14 shows that a plot of g_L versus $(L/\xi)^2 \propto L^2\left(\frac{T}{T_c}-1\right)$, the standard finite size scaling variable, is much less successful. As expected, there is no data collapsing with this choice of variables, and particularly, the data for $L=5, 6, 7$ still systematically deviate from each other. In this representation, g_L converges for $L\to\infty$ against a step function at T_c as the original data do (Fig. 4); of course, the slope at T_c increases only rather slowly now (proportional to an exponent 5/4 of the chosen variable, $(L^2)^{5/4}=L^{5/2}$).

V. Conclusions

In this paper both the bulk critical behaviour and finite size scaling for the five-dimensional Ising model were analyzed, using Monte Carlo data for systems in the size range $N=3^5=243$ to $N=7^5=16807$. Of course, due to these very small linear dimensions the regime very close to criticality was not accessible to study. Although with more sophisticated programs on vector computers or special purpose Monte Carlo processors one could go to considerably larger values of N, in terms of the linear dimension L it would mean at best an increase of a factor of two or three for this high-dimensional system; thus one still would somewhat suffer from the same problems. Nevertheless, such an extension of the present work would be very desirable.

In spite of this intrinsic limitation we feel that useful results have been obtained, involving the known critical exponents of Landau theory for the leading terms, and focusing on the singular correction terms to this behaviour, as well as on finite size scaling. Above T_c the estimated susceptibility agrees quantitatively with the series extrapolation due to Guttmann, Eq. (11); a corresponding square-root singularity was also identified for the specific heat, where such a term is expected on general theoretical grounds, but has not yet been studied by series expansions. While correction terms clearly are also rather important for the magnetization, the data seem to favor a less singular correction, Eq. (15).

The present analysis of finite size effects of this model confirms the conclusion of [14], that the shift of the effective critical temperature $\Delta T_c=T_c(L)-L \propto L^{-y_T^*}=L^{-5/2}$, rather than the standard relation $\Delta T_c \propto L^{-1/\nu}(=L^{-2}$ in this model). Thus both rounding and shifting of critical singularities in this model do not occur when L is comparable to the correlation length, but rather when L is comparable to the (smaller) "thermodynamic length" $l\propto|1-T/T_c|^{-1/y_T^*}$. We hope that the present analysis may also be useful for other problems where either d exceeds the marginal dimensionality d^*, or hyperscaling is violated because of other reasons.

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