We employ the recently proposed scaling theory for first-order transitions to derive a detailed prediction for the large-argument behaviour of the critical-point scaling function of the reduced fourth order cumulant $g_L = \langle s^4 \rangle / \langle s^2 \rangle^2 - 3$ correct up to a term exponentially small in $L/\xi(T)$.

Recently, extensive Monte Carlo (MC) calculations have been performed for the $(d = 3)$-dimensional Ising model on $L \times L \times L$ simple cubic lattice of up to $N = (L/a)^3 \leq (128)^3$ sites. (Here $a$ denotes the lattice spacing.) The numerical studies of refs. 1, 2, 4 have concentrated on the reduced fourth order cumulant

$$g_L(T) = \langle s^4 \rangle / \langle s^2 \rangle^2 - 3 |_{h=0} = [\chi_L^{(4)} L^{-d} \chi_L^{-2}] |_{h=0},$$

where

$$s = N^{-1} \sum_{i=1}^{N} s_i,$$

$$\chi_L = - \frac{\partial^2 f_L}{\partial h^2} \quad \text{and} \quad \chi_L^{(4)} = - \frac{\partial^4 f_L}{\partial h^4}.$$

Here the reduced free-energy density is defined via

$$f_L = -L^{-d} \ln \left\{ \sum_{s_{i_{1} \neq \ldots \neq s_{i_{N}}}} \sum_{s_{j_{1} \neq \ldots \neq s_{j_{N}} = \perp}} \left[ \exp \left( K \sum_{n.n.} s_i s_j + h \sum_i s_i \right) \right] \right\}, \quad K = J/k_B T.$$

The function, $g_L(T)$, introduced by Binder, has become increasingly popular in MC studies.

In this note we consider the finite-size scaling behaviour near $T_c$ with an emphasis on those properties which may be inferred from the fact that the $h = 0$, $T < T_c$ phase boundary should be controlled by the $T = 0$ discontinuity.
fixed point\(^6\)). Thus the critical scaling functions should exhibit crossover\(^7\) to the first-order scaling forms which have been derived recently\(^7-9\)) by a combination of scaling arguments, sum rules, and transfer matrix techniques. For definiteness, we consider only \(L^d\) hypercubic samples with periodic-type (i.e. periodic, screw-periodic, etc.) boundary conditions. These, of course, are the normal choice in MC Studies. Then the finite-size scaling relation for the singular part of the free-energy density can be written\(^5,7,10\) as

\[
f_L(t) = L^{-d} E\left(t L^{d/(2-\alpha)}, h L^{d/2-\alpha}\right), \quad t \equiv (T - T_c)/T_c,
\]

where \(d/(2-\alpha)\) can be replaced by \(1/v\) if hyperscaling holds: see the discussion in ref. 10. The exponents \(\alpha\) and \(\Delta = \beta + \gamma\) describe the bulk thermodynamic behaviour as usual\(^5\). For \(g_L(T)\), which is considered only for \(h = 0\), we have

\[
g_L(T) = G(t L^{d/(2-\alpha)}).
\]

There are various approaches\(^7-\alpha\)) to first-order scaling, but all predict that for \(|h| \ll (m_b \xi_b)^{-1} L^{1-d}\) and \(L \gg \xi_b\), one should expect

\[
f_L(h, T < T_c) = f_d(0, T < T_c) + L^{-d} \ln 2 \approx -L^{-d} \ln \cosh(m_b h L^d),
\]

so that

\[
m_L(h, T < T_c) = m_b \tanh(m_b h L^d),
\]

e tc. Here and below the subscript \(b\) denotes the bulk ‘spontaneous’ or ‘initial’ values calculated with the limit \(L \to \infty\) taken before \(h \to 0\). For large \(L\), there is a region in which the scaling forms (4) and (6) overlap\(^7\). If both expressions are to be valid, this implies restrictions on the limiting form of critical scaling functions, see ref. 7. Indeed, the first-order scaling relation (7) implies, after some algebra, that \(G(x)\) in (5) should satisfy \(\lim_{x \to -\infty} G(x) = -2\). Actually, this result is implicit in (1) and is rather straightforward to derive.\(^4\)

In order to obtain a more detailed prediction, namely relation (13) below, for the behaviour of \(G(x)\) for large negative \(x\), we may consider corrections to the leading first-order scaling forms. The leading scaling relations\(^7\), (6), (7), etc. can be derived\(^4,7-\alpha\), completely or in part, by various approaches which, when combined, are rather convincing. However, the status of corrections to these leading scaling relations is less satisfactory. One approach, which applies only to systems with periodic-type boundary conditions, has been outlined in ref. 7 where \(\chi_L\) was found to behave as

\[
\chi_L(|h| \ll (m_b \xi_b)^{-1} L^{1-d}; T < T_c) = L^d m_b^2 \cosh^{-2}(m_b h L^d) + \chi_0 + O(h, e^{-L/\xi_b}).
\]

\[\hfill (8)\]
The derivation of this result is based on various phenomenological observations\(^\text{2,11}\) regarding the structure of the spectrum of a transfer matrix and employs properties of the so-called 'single-phase free energy functions' introduced in refs. 11. The results are nonrigorous and are therefore open to challenge; however, similar relations can also be derived\(^\text{4,9}\) by assuming a two-peak property of the probability distribution, \(P(s)\), for the values of \(s = N^{-1} \sum_{i=1}^{N} s_i\); below \(T_c\) one expects \(P(s)\) to have relatively sharp maxima at \(s \approx \pm m_b\). However, this derivation involves somewhat arbitrary manipulations of interchanging \(\langle s \rangle^2, \langle s \rangle^2, \langle |s| \rangle^2\), in order to obtain finite quantities in taking the two noncommuting limits \(h \rightarrow 0^+\) and \(L \rightarrow \infty\) in different orders. The transfer matrix analysis\(^\text{2,11}\) provides a more controlled procedure especially when residual corrections, like \(O(e^{-L/d})\) in (8), are required.

With the reservations mentioned in mind, we may extend the calculations of ref. 7 to obtain expressions for \(\chi_L^{(6)}(h = 0, T < T_c)\) and \(g_L(T)\) for \(T < T_c\). We use the representation\(^\text{7}\),

\[
f_L(h, T) = \frac{1}{2}(f_+ + f_-) - V^{-1} \ln 2 \cosh \left[ \frac{1}{2} V(f_+ - f_-) \right] + O(e^{-L/d^2}),
\]

valid for \(|h| \ll (m_b \xi_b)^{-1} L^{-d}\) and \(L \gg \xi_b\), where \(f_\pm\) denote the single phase free energy functions\(^\text{11}\) which, in (9), can be replaced\(^\text{7,11}\) by bulk, asymptotic power series in \(h\), namely

\[
f_\pm = f_b \mp m_b h - \frac{1}{2} \chi_b h^2 + \frac{1}{8} \chi_b^{(3)} h^3 - \frac{1}{24} \chi_b^{(4)} h^4 + O(h^5).
\]

We have put \(\chi_b^{(3)} = -\partial^3 f_b / \partial h^3\), in analogy with \(\chi_b^{(4)}\).

A tedious, but straightforward calculation of \((\partial^4 f_L / \partial h^4)_{h=0}\) gives

\[
\chi_L^{(4)}(h = 0, T < T_c) = -2 m_b L^{3d} + 4 m_b \chi_b^{(3)} L^d + \chi_b^{(4)} + O(e^{-L/d^2}).
\]

Similar formulae for \(\chi_L^{(6)}\) and \(\chi_L^{(8)}\) are given in appendix A. From (8) and (11), we find

\[
g_L(T) = \frac{-2 m_b^4 L^{3d} + 4 m_b \chi_b^{(3)} L^d + \chi_b^{(4)}}{L^d (L^d m_b^4 + \chi_b^{(3)})^2} + O(e^{-L/d^2}) \quad \text{for } T < T_c.
\]

Finally, by comparing (12) with the critical scaling form (5) we obtain a prediction for \(G(x)\) in the domain of large negative-\(x\), namely

\[
G(x) = \frac{-2 a_1 |x|^{2a} + 4 a_1 a_2 |x|^{2a} + a_2^2}{|x|^{2a} (a_1^2 |x|^{2a} + a_2^2)^2} + \epsilon(x),
\]
as \( x \to -\infty \), where \( \varepsilon(x) \) denotes terms exponentially small as \( |x| \to \infty \) and we have introduced bulk critical amplitudes defined via

\[
m_b \approx a_1 \|t\|^\mu, \quad \chi_b \approx a_2 \|t\|^{-\gamma}, \quad \chi_b^{(3)} \approx a_3 \|t\|^{-\gamma-\delta}, \quad \chi_b^{(4)} \approx a_4 \|t\|^{-\gamma-2\delta},
\]

for \( t \to 0^- \). Verification of (13) by numerical studies would be of interest as confirmation of the phenomenological methods\(^4,7,9\) by which relations of this type have been derived.

Notice that the relation (12) should be valid for \( T > T_c \) as well, provided \( L \gg \xi_b \); indeed, \( m_b \) and \( \chi_b^{(3)} \) vanish for \( T > T_c \), so that (12) follows directly from (1) and the observation\(^5\) that for periodic boundary conditions the rate of convergence of non-critical quantities to the bulk values is like \( e^{-L/\xi_b} \). For positive \( x \geq 1 \), one thus expects

\[
G(x) = \frac{a_4^+}{(a_2^+) \frac{2}{x}} + \varepsilon(x), \quad \text{as } x \to +\infty,
\]

where \( a_4^+ \) are defined with \( t \to 0^+ \) in (14).

In summary, we have derived a rather detailed prediction, relation (13), for the critical point finite-size scaling properties of the cumulant \([\langle s^4 \rangle / \langle s^2 \rangle^2 - 3]\), which is implied by the crossover to first-order scaling\(^7\) along the phase boundary below \( T_c \).

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**Appendix A**

Various quantities constructed from higher-order derivatives of the free-energy density are of interest\(^4,7,12\) in finite-size scaling. We list here, for reference, formulae for \( \chi^{(6)} = -\delta^6 f / \partial h^6 \) and \( \chi^{(8)} = -\delta^8 f / \partial h^8 \) at the phase boun-
These expressions have been derived by using the computer program MACSYMA:

\[
\chi_L^{(6)}(h = 0, T < T_c) = 16m_b^6L^{5d} - 40m_b^3\chi_b^{(3)}L^{3d} \\
+ (10\chi_b^{(3)} + 6m_b\chi_b^{(5)})L^d + \chi_b^{(6)} + O(e^{-L/\xi}), \quad (A.1)
\]

\[
\chi_L^{(8)}(h = 0, T < T_c) = -272m_b^8L^{7d} + 896m_b^5\chi_b^{(3)}L^{5d} \\
- (112m_b^3\chi_b^{(5)} + 560m_b^2\chi_b^{(3)})L^{3d} \\
+ (56\chi_b^{(3)} + 8m_b\chi^{(7)})L^d + \chi_b^{(8)} + O(e^{-L/\xi}). \quad (A.2)
\]

References

2) M.N. Barber, R.B. Pearson, D. Toussaint and J.L. Richardson, NSF-ITP 83-144 (to be published).