Monte Carlo Studies of Correlation Length and Hyperscaling in the Three-Dimensional Ising Model

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We report extensive Monte Carlo simulations and finite-size scaling analysis of the correlation length (ξ_L) for the spin-spin correlation function and the renormalized coupling (g_L) of the simple-cubic Ising model with a wide range of lattice sizes ($L \leq 96$). New methods of analysis which avoid assumptions related to the correlation length were introduced. The exponents ν and $2-\alpha$ were estimated from separate analysis of ξ_L and g_L, respectively. A value of $\omega^* \approx 0.001 \pm 0.07$ for the Fisher exponent is obtained. This is consistent with very small or no violation of hyperscaling.

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The theory of critical phenomena provides a detailed description of the properties of a physical system near the critical point in terms of scaling and a set of critical exponents.[1,2] These exponents are universal for systems in a given universality class. Only the spatial dimension and the symmetry of the interactions enter in the classification of universality class. For a given universality class, these exponents are not independent, but are related to each other by various proposed exponent equalities and inequalities. One particular set of exponent relations, the hyperscaling relations, involves the spatial dimension.[3] This is of some importance because it enters in renormalization-group theory,[4,5] which has been able to provide a detailed physical understanding of critical phenomena. The possibility of hyperscaling violation thus has broad fundamental implications. Failure of hyperscaling for model systems in more than four dimensions are well established.[5,6] For soluble two-dimensional models, such as the Ising model,[7] hyperscaling is obeyed exactly. In the physically interesting dimension of three, with the absence of exact solutions, the validity of hyperscaling has been subjected to extensive discussions and considerable research.[5,6,8–17]

Two numerical methods that have contributed to the study of hyperscaling for three dimensions are series expansions and Monte Carlo simulations. The series method produces accurate results for the system in the thermodynamic limit and is only limited by the length of the series and the method of analysis. Early series-expansions results have been conflicting,[8–12] but more recent studies[13,14] are consistent with each other. In particular, one study[13] indicated that there are no grounds for doubting that the three-dimensional spin-$\frac{1}{2}$ Ising model obeys hyperscaling. In contrast, the applications of the Monte Carlo method have been more inconclusive.[15,16] Previous simulations are significant and very useful, focusing attention on the possibility of applying the Monte Carlo methods. In principle, this method provides numerically exact results on finite lattices. The limitations to the method are the need for sufficiently large lattices to probe the asymptotic scaling regime and good sampling statistics. The quantities measured in the simulations must also be able to provide an unambiguous test of the hyperscaling relations without unnecessary assumptions.[17] Previous simulations have been constrained by at least one of these limitations.[17]

In this paper, we report on extensive Monte Carlo simulations and finite-size scaling analysis on the correlation length of the spin-spin correlation function and the renormalized coupling for the nearest-neighbor ferromagnetic Ising model on the simple-cubic lattice. A wide range of lattice sizes and temperatures near T_C were used to produce the data, which were then analyzed with the assumption that possible violations are due to dangerous irrelevant variables. An estimate for the Fisher exponent was obtained. Furthermore, a previously proposed method of analysis, involving the scaling properties of the renormalized coupling at a fixed ratio of the correlation length to the lattice size, was also used to obtain another estimate for the Fisher exponent. The results of both methods are consistent with very small or no hyperscaling violation.

Finite-size scaling of the correlation length and the renormalized coupling.— One theoretical argument for conceivable hyperscaling violation in models of the three-dimensional Ising universality class is the possible existence of a dangerous irrelevant variable.[5,6] Although, so far there has been no rigorous evidence for such a variable, the consequence of its presence in regard to hyperscaling violations has been explored in some detail.[5,6,17] In this paper, we will only quote those theoretical results related to the finite-size analysis of our simulation data. The reader is referred to the original papers for details.

Consider the finite-size scaling[18] of the singular part of the free energy f_L and the correlation length ξ_L,[17]

$$f_L = L^{-d} f(tL^{y_T}, hL^{y_H}, uL^{y_U}) , \tag{1}$$

$$\xi_L = L\xi(tL^{y_T}, hL^{y_H}, uL^{y_U}) , \tag{2}$$

where d is the dimension, t is the reduced temperature $t=(T-T_C)/T_C$, h is the magnetic field, and u is the irrelevant variable. Care must be taken in the choice of the definition for the correlation length of a finite system;[17,18] the second moment of the correlation function is considered here. Assuming that u is a dangerous irrelevant variable, one obtains

$$f(x,y,z)=z^{p_1}\bar{f}(xz^{p_2},yz^{p_3})\,, \tag{3}$$

and

$$\xi(x,y,z)=z^{q_1}\bar{\xi}(xz^{q_2},yz^{q_3})\,. \tag{4}$$

These equations imply the following:

$$f_L=L^{-d}F(tL^{y_T^*},hL^{y_H^*})\,, \tag{5}$$

with $y_T^*=y_T+p_2y_U$ and $y_H^*=y_H+p_3y_U$;

$$\xi_L(t,h)=L^{1+q_1y_U}z(tL^{y_T^{**}},hL^{y_H^{**}})\,, \tag{6}$$

where $y_T^{**}=y_T+q_2y_U$ and $y_H^{**}=y_H+q_3y_U$. The correlation-length exponent is related by

$$\nu=(1+q_1y_U)/y_T^{**}\,. \tag{7}$$

A measure of hyperscaling violation[6] is given by the Fisher exponent ω^*. For the cubic-shaped system used in our simulations, it was shown that[17]

$$\omega^*=d(1-1/\nu y_T^*)\,. \tag{8}$$

This vanishes exactly if hyperscaling is obeyed.

To test hyperscaling without further assumptions, one only needs to estimate ν from the finite-size scaling properties of ξ_L and y_T^* from f_L or the renormalized coupling g_L introduced by Binder,[19]

$$g_L=\langle s^4\rangle_L/\langle s^2\rangle_L^2-3\,. \tag{9}$$

For $h=0$ and T near T_C this takes the form

$$g_L(t)=G(tL^{y_T^*})\,. \tag{10}$$

$2-\alpha$ can now be obtained from $y_T^*=d/(2-\alpha)$. We have estimated ν in two steps. First, we consider any two sets of (t_1,L_1) and (t_2,L_2) such that

$$R(L_1,t_1)=R(L_2,t_2)\,, \tag{11}$$

where

$$R(L,t)\equiv\xi_L(t)/\xi_L(t=0)=Z(tL^{y_T^{**}})/Z(0)\,.$$

We obtain

$$y_T^{**}=\frac{\ln(t_1/t_2)}{\ln(L_2/L_1)}\,. \tag{12}$$

This can be considered as an adaptation of the "matching method," previously introduced to analyze Monte Carlo data in another context.[20] Second, an estimate of $1+q_1y_U$ is obtained from the L dependences of $\xi_L(t=0)$; see Eq. (6). The value of T_C can, in principle, be obtained as a fitting parameter, such that the "matching" is successful. In practice, we started out with the value of $J/k_BT_C=0.221\,655$.[21] The uncertainty in T_C is in the last digit. We have varied our T_C within ten times the uncertainty of Ref. 21 and our results remain the same within our statistical errors. To measure y_T^*, we can also use the matching method on Eq. (10) or use the following relation:

$$y_T^*=\frac{\ln\{[dg_{bL}(t=0)/dt]/[dg_L(t=0)/dt]\}}{\ln b}\,, \tag{13}$$

where $dg_L(t=0)/dt$ is the derivative of g_L with respect to t at $t=0$. b is a scale factor.

A much simpler method of analysis which does not depend on the precise value of T_C was previously used by Freedman and Baker.[15] However, they need implicitly the assumption[17] that $q_1y_U=0$ and then choose values of $t>0$ for which $\xi_L(t)/L=\text{const}$. The finite-size scaling properties become,

$$g_L(t)\sim L^{-\omega^*}\,. \tag{14}$$

ω^* is estimated from this finite-size dependence.

Monte Carlo method.—We have adopted the definition of the correlation length used by Binder *et al.*,[17]

$$2d\xi_L^2=\frac{\sum_{i,j}(r_i-r_j)^2(\langle s_is_j\rangle-c_L)}{\sum_{i,j}(\langle s_is_j\rangle-c_L)}\,, \tag{15}$$

where r_i is the position of lattice site i,

$$c_L=(1/L^d)\sum_i\langle s_is_{i'}\rangle\,,$$

and i' is the site with $r_{i'}=r_i+\frac{1}{2}(1,1,1)L$. A modified version of the very fast multispin vectorized Monte Carlo code[22] on the Cyber 205 supercomputer was used for a wide range of lattice sizes ($L\le 96$) and up to five million Monte Carlo steps per spin. Different runs (typically five) were used to estimate the statistical errors. We have ensured that our runs are sufficiently long to overcome critical slowing down for the system sizes and temperatures considered. Our results were also checked

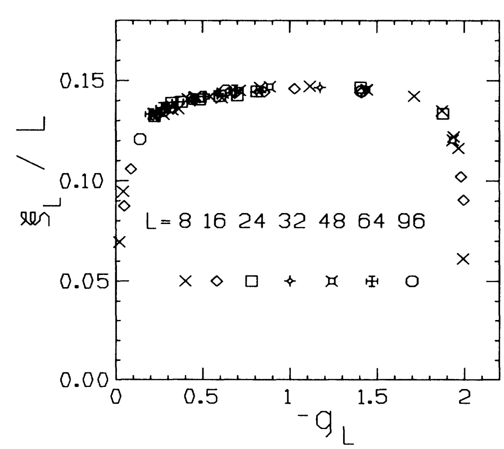

FIG. 1. Scaling plot of the ratio $\xi_L(t)/L$ vs the renormalized coupling $g_L(t)$.

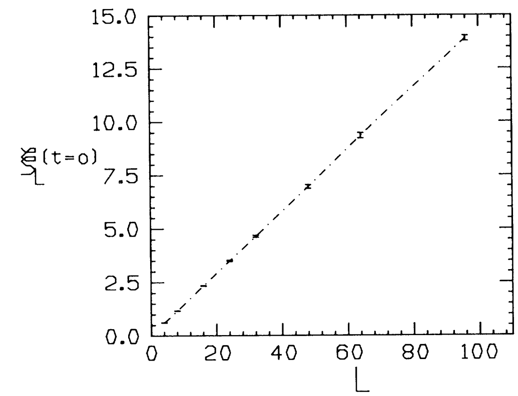

FIG. 2. Plot of the correlation length at criticality vs the size of the system. The dashed-dotted line is a least-squares fit for the $L \geq 16$ data. See text.

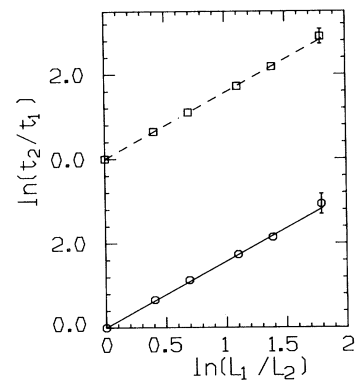

FIG. 3. Example of log-log plot of the ratio t_2/t_1 vs L_1/L_2. $L_2=16$ and $t_2=0.03$. The squares are for g_L and the circles for ξ_L. The lines are least-squares fits and the slopes give estimates for the exponents. See text.

against published[15,16,19,23] Monte Carlo values for the g_L. The correlation-length data for large values of $tL^{1/\nu}$ were compared with series-expansion estimates.[24] The agreements are very satisfying and full details will be reported elsewhere.

Results.—The data for the correlation length and renormalized coupling were analyzed with finite-size scaling. First, we present the data as a universal scaling plot by plotting $\xi_L(t)/L$ vs $g_L(t)$ for $L \geq 8$; see Fig. 1. The data scale very well, indicating that our data are in the scaling regime and both $q_1 y_U$ and ω^* are very small. For quantitative analysis, we have implemented the two methods discussed above. From Eq. (6), we obtained by least-squares fits for the large-L data ($L \geq 16$) an estimate of $q_1 y_U = -0.0036 \pm 0.006$. This is indeed very close to zero; see Fig. 2. We have systematically excluded the smaller-size data in our fits and the estimates remain constant within the errors. To apply the matching method, we have fitted both the function $R(L,t)$ [for $\xi_L(t)$] and $g_L(t)$ with polynomials. For fixed values of L_1, L_2, and t_2, we obtain numerically the zero of the function $H(t_1)=R(L_1,t_1)-R(L_2,t_2)$. A similar procedure is used for $g_L(t)$. The exponents are estimated with Eq. (12) by plotting t_2/t_1 vs L_1/L_2 on a log-log plot; see Fig. 3. We obtain by least-squares fits $y_T^* = 1.578 \pm 0.016$ and $y_T^{**} = 1.57 \pm 0.02$, or $\alpha = 0.10 \pm 0.02$ and $\nu = 0.634 \pm 0.01$. The errors are estimated by using different combinations of L_1 and L_2 and are orders of magnitudes larger than the changes produced by the uncertainty in T_C. These values give $\omega^* = 0.001 \pm 0.07$. y_T^* can also be obtained from the temperature derivative of the renormalized coupling constants at $t=0$; see Eq. (13). To use this method, we have analyzed our data for $L \geq 16$. We obtained $y_T^* = 1.584 \pm 0.03$ and $\omega^* = 0.01 \pm 0.10$.

To implement the method of Freedman and Baker,[15] we have chosen various values for the ratio $\xi_L(t)/L$ and fitted the data according to Eq. (14); see Fig. 4(a). The distributions of ω^* obtained by least-squares fits are given in Fig. 4(b). The estimate for the average value is 0.015 ± 0.02.

Discussions.—We have presented extensive Monte Carlo simulations and separate finite-size scaling analysis of the correlation length and the renormalized coupling. The matching method of analysis was adopted. This produces a very small estimate for the Fisher exponent of $\omega^* = 0.001 \pm 0.07$ in agreement with the result $\omega^* = 0.015 \pm 0.02$, obtained by using the method of Freedman and Baker. Thus, these new Monte Carlo results are consistent with the more recent series-expansion result $\omega^* = 0.001 \pm 0.010$.[13] Although the accuracy is lower than that of the series expansion, our results are

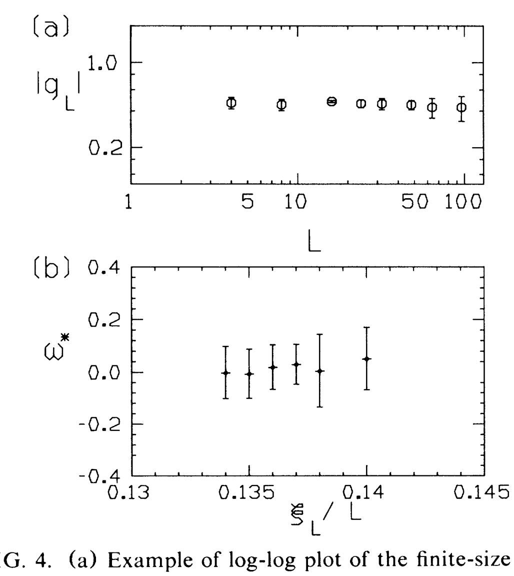

FIG. 4. (a) Example of log-log plot of the finite-size dependences of the renormalized coupling vs the size for the fixed value $\xi_L/L = 0.14$. (b) Estimates for the Fisher exponent with the method of Freedman and Baker for a range of ξ_L/L.

significant. We exhibit here clearly for the first time that reliable estimates of the amount of hyperscaling violation can be obtained from the Monte Carlo methods. There is little doubt that the statistics can be further improved. We have made no attempts to reduce the sampling errors with various recently proposed techniques to reduce the critical slowing down.[25-27] These are nontrivial to apply with the vectorized multispin coding, but will increase the efficiency and accuracy considerably. They should be implemented in further studies.

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[1]See reviews in, *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1984), Vols. 1–9.

[2]M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967).

[3]M. E. Fisher, in *Collective Properties of Physical Systems (Nobel Symposium 24),* edited by B. Lundqvist and S. Lundqvist (Academic, New York, 1974).

[4]For reviews see, K. G. Wilson and J. B. Kogut, Phys. Rep. **12C**, 75 (1974).

[5]M. E. Fisher, in *Advanced Course on Critical Phenomena,* edited by F. J. W. Hahne, Lecture Notes in Physics Vol. 186 (Springer-Verlag, Berlin, 1983).

[6]M. E. Fisher, in *Renormalization Group and Quantum Field Theory,* edited by J. D. Gunton and M. S. Green (Temple University, Philadelphia, 1974).

[7]L. Onsager, Phys. Rev. **65**, 117 (1944).

[8]G. A. Baker, Jr., Phys. Rev. B **15**, 1552 (1977).

[9]B. G. Nickel and B. J. Sharpe, J. Phys. A **12**, 1819 (1979).

[10]J. J. Rehr, J. Phys. A **12**, L179 (1979).

[11]C. Domb, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

[12]B. G. Nickel, in *Phase Transitions Cargese 1980,* edited by M. Levey, J. C. Leguillou, and J. Zinn-Justin (Plenum, New York, 1982).

[13]M. E. Fisher and J.-H. Chen, J. Phys. (Paris) **46**, 1645 (1985).

[14]A. J. Guttmann, Phys. Rev. B **33**, 5089 (1986).

[15]B. A. Freedman and G. A. Baker, Jr., J. Phys. A **15**, L715 (1982).

[16]M. N. Barber, R. B. Pearson, D. Toussaint, and J. L. Richardson, Phys. Rev. B **32**, 1720 (1985).

[17]K. Binder, M. Nauenberg, V. Privman, and A. P. Young, Phys. Rev. B **31**, 1498 (1985).

[18]V. Privman and M. E. Fisher, J. Stat. Phys. **33**, 385 (1983). For reviews, see, M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8.

[19]K. Binder, Z. Phys. B **43**, 119 (1981).

[20]S. Shenker and J. Tobochnik, Phys. Rev. B **22**, 4462 (1980).

[21]G. Pawley, R. H. Swendsen, D. J. Wallace, and K. G. Wilson, Phys. Rev. B **29**, 4030 (1984).

[22]S. Wansleben, J. Comput. Phys. Comm. **43**, 315 (1987).

[23]G. Bhanot, D. Duke, and R. Salvador, Phys. Rev. B **33**, 7841 (1986).

[24]A. J. Liu and M. E. Fisher, Physica (Amsterdam) (to be published); H. B. Tarko and M. E. Fisher, Phys. Rev. B **11**, 1217 (1975).

[25]R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).

[26]J. Goodman and A. D. Sokal, Phys. Rev. Lett. **56**, 1015 (1986).

[27]D. Kandel, E. Domany, D. Ron, A. Brandt, and E. Loh, Jr., Phys. Rev. Lett. **60**, 1591 (1988).