Renormalized Coupling Constant for the Three-Dimensional Ising Model

George A. Baker, Jr., and Naoki Kawashima*
Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico 87544
(Received 13 December 1994)

Monte Carlo calculations of the renormalized coupling constant for the three-dimensional Ising model are reported. Improved estimators both for the second partial of the susceptibility with respect to the magnetic field and for the correlation length are developed. These estimators show greatly improved convergence properties, and allow us to compute for system sizes and temperature rather more relevant to the thermodynamic limit than previously. Our results indicate strongly that hyperscaling holds for this model.

PACS numbers: 05.50.+q, 02.70.Lq, 05.70.Jk, 75.10.Hk

The modern theory of critical phenomena has been troubled since its earliest days when scaling theory was introduced [1] with the problem of the validity of those relations between the critical indices which involve the spatial dimension. As Stell [2] pointed out, and as was later incorporated in a theoretical structure by Fisher [3] as the "anomalous dimension of the vacuum" ω^*, the ideas of scaling and homogeneity are compatible with the replacement of the spatial dimension d by $d - \omega^*$. Thus the ideas of scaling alone do not require these "hyperscaling relations." We do know, however, as Schrader [4] and Baker and Krinsky [5] have shown, that $\omega^* \geq 0$. With the introduction of the more powerful ideas of the renormalization group by Wilson [6], and particularly the field theory approach [7], these hyperscaling relations became an integral part of the theory. During the period before the renormalization group theory (and continuing still), the only really quantitative method to obtain accurate predictions of the critical properties was the method of the analysis of exact perturbation series. Unfortunately, the best estimates from the high-temperature series showed just barely resolved violations of the hyperscaling [8].

The key parameter in the renormalization group theory is the renormalized coupling constant. It is defined (for zero reduced magnetic field $H = \beta m h$, where h is the magnetic field, m is the magnetic moment, and $\beta = 1/kT$ with k Boltzmann's constant) as

$$g^* = \lim_{K \to K_c^-} g(K) = - \lim_{K \to K_c^-} \frac{\partial^2 \chi(K)/\partial H^2}{\chi^2(K) \xi^d(K)}, \quad (1)$$

where K_c is the critical value of the inverse temperature $K = \beta J$ with J the exchange energy, χ is the magnetic susceptibility, and ξ is the second-moment definition correlation length. The value of this constant derived by the field theory implementation of the renormalization group [9] is $g^* = 23.73 \pm 0.02$. Recently Tamayo and Gupta [10] have computed by Monte Carlo methods a value of $g^* = 6$–7 for the limit as the system size goes to infinity of $g(K_c = 0.221\,655)$. There is a significant amount of difference between these two results. Previous series studies [11,12] had found by series analysis that the value of $g(K)$ was dropping sharply, as $K \to K_c$, and suggested that $g^* = 0$. If that result is correct, it could imply a violation of the hyperscaling relations. Earlier Monte Carlo studies [13] indicate values declining below the field theory value as $K \to K_c^-$. A special computer was built [14] to attempt to resolve this issue, but unfortunately it was built to compute the wrong quantity [15].

There have been several complicating factors which have conspired to delay the resolution of this question. First, it now appears that the effects of the complex nonanalytic structure of $g(K)$ near $K = K_c$ is more severe than expected from the relatively mild problems observed in the analysis of the susceptibility. This problem has disrupted accurate series analysis. Further, the problem of critical point "rounding" in the finite size theory of $g(K, L)$, where L is the system size, has only recently [16] been appreciated. It turns out that $(K = K_c, L = \infty)$ is a point of nonuniform approach. Baker [17] has demonstrated this effect in the two-dimensional Ising model through *exact* calculations on squares of size $L \leq 10$. There the limits of $g(K, L)$ as $K \to K_c$ and $L \to \infty$ do not appear to commute. Further evidence on this point could be the differences between Tamayo-Gupta [10] results and the field theory results cited above. There is a further complicating factor. In the three-dimensional Ising model Baker and Erpenbeck [16] have obtained good data collapse for $g(K, L)(K/K_c)^{1.5}$ vs $\xi_L(K)/L$, where $\xi_L(K)$ is the correlation length computed on the L cube. Their results indicate clearly that computations using $\xi_L/L \geq 0.26$ are unsatisfactory for the computation of the thermodynamic limit and will give values which are too small. This result throws in question the results of Ref. [13]. Between these two effects, all the previous Monte Carlo estimates, of which the authors are aware, are inadequate to clearly resolve this problem. A further complication which arises when one tries to reduce the value of ξ/L is that cancellations occur in the computation of $\partial^2 \chi/\partial H^2$ from the subtraction of two terms which are of order $(L/\xi_L)^d$ larger than the answer. It is for this reason that a calculation [10,16] at $K = K_c$ where $\xi_L/L \approx 0.6$ is much easier than for the values required to give the thermodynamic limit.

 0031-9007/95/75(6)/994(4)$06.00

In this Letter we report a set of Monte Carlo results. We have derived new estimators for both ξ^2 and $\partial^2\chi/\partial H^2$ which have much better convergence properties. These estimators are key to obtaining our results without the use of much greater computer resources. We have obtained results for $g(K)$ for a sequence of temperatures and system sizes such that $\xi/L \approx 0.1$. This value seems to be small enough to assure that our results agree with the thermodynamic limit within 1%. We emphasize that the quantities which we are computing are the self-same ones calculated by series analysis, and, if one accepts the renormalization group hypothesis, the ones calculated by field theory methods. The only difference comes from the possible systematic error of selecting $\xi/L > 0$. We conclude that the value of g^* is nonzero and so hyperscaling should hold for the three-dimensional Ising model. It is probable that $g(K)$ displays an inverted cusp at the critical point.

For our computations, we used the Swendsen-Wang algorithm [18] for spin updating. This type of algorithm has two advantages over the conventional algorithm, i.e., reduction in the autocorrelation time, and reduction in the variances of equilibrium distributions of relevant quantities. As has been reported by several authors [19], we observed that the cluster algorithm with improved estimators dramatically reduces statistical errors. It was reported [20] that cluster algorithms are not much more efficient than conventional algorithms with multispin coding technique when only the benefit from correlation-time reduction is taken into account. We emphasize, however, that not only reduction of the correlation times but also use of improved estimators was crucial to the present work. In fact, our preliminary computation showed that, for the 64 cube, it was impossible to obtain results as accurate as the ones presented in this Letter by means of a conventional algorithm within a reasonable computational time ($\sim$ a few months) and within the given resources, at the temperatures of the present interest. (Our computations were mainly performed on a cluster of eight IBM RS/6000 model 590's. But some were done on a SUN Sparcserver 2000.) As we will show, even for smaller lattices, it was obvious that the cluster algorithm performs better.

To extract the full potential of the cluster algorithm, we reexpressed all the quantities that need to be computed in terms of improved estimators. Our goal is to calculate the renormalized coupling constant (1) which is related to the magnetic moments by

$$g \equiv \left(\frac{L}{\xi}\right)^d \frac{3\langle M^2\rangle^2 - \langle M^4\rangle}{\langle M^2\rangle^2}. \tag{2}$$

Here, $\chi \equiv \langle M^2\rangle/N$ where M is the total magnetization and $N \equiv L^d$ is the number of lattice sites. From (2), it is clear that we have to calculate three quantities: the second and the fourth moments of the magnetization and the correlation length.

It is well known that an improved estimator for the second moment of magnetization is simply the average size of clusters [21], i.e.,

$$\langle M^2\rangle = \left\langle \sum_c V_c^2 \right\rangle. \tag{3}$$

Here, V_c is the number of sites in a cluster c. The practical point of estimators of this type is that the cluster-cluster terms, which should be zero, are automatically zero, and do not have to be estimated, which greatly speeds the Monte Carlo convergence. For the fourth moment of magnetization, we can derive by the same methods the corresponding estimator,

$$\langle M^4\rangle = 3\left\langle \left(\sum_c V_c^2\right)^2 \right\rangle - 2\left\langle \sum_c V_c^4 \right\rangle. \tag{4}$$

For the correlation length, we used [22]

$$f(\vec{k}) \equiv 4\sin^2\left(\frac{\vec{k}}{2}\right)\left(1 - \frac{\chi(\vec{k})}{\chi}\right)^{-1} \tag{5}$$

as an approximant to ξ^{-2} in the zeroth order with respect to $|\vec{k}|$. Here $\chi(\vec{k}) \equiv \langle |M(a\vec{k})|^2\rangle/N$, where $M(\vec{k})$ is defined by $M(\vec{k}) = \sum_{\vec{r}} \exp(-i\vec{k}\cdot\vec{r})S_{\vec{r}}$. In the actual calculation, we formed a linear combination of $f(\vec{k})$ with the six smallest possible values of $|\vec{k}|$, which correspond to the nearest and second nearest neighbors to the origin in the reciprocal space, so that the correction term of the second order in $|\vec{k}|$ cancels out in the case where it is isotropic. Therefore, our approximant is of the second order in $1/L$ with this assumption, besides the error due to the finite size effect. We can express $\chi(\vec{k})$ in a fashion similar to (3) simply by replacing V_c in (3) by $V_c(\vec{k}) \equiv |\sum_{\vec{r}\in c} \exp(i\vec{k}\cdot\vec{r})|$. Thus, we have expressed all the necessary quantities in terms of improved estimators.

Our simulation consists of N_S independent sets of runs. Each run is divided into first, N_E sweeps for equilibration, followed by N_M Monte Carlo sweeps for measurement. Each measurement sweep is, however, followed by n_R sweeps to improve independence before the next measurement step. Therefore the total number of Monte Carlo sweeps performed is $N_S[N_E + (n_R + 1)N_M]$. Only in the conventional algorithm is it necessary to take $n_R > 0$. In the conventional algorithm, namely, the item marked by (a) in Table I, N_E refers only to the first coarse grained sample, so the total number of Monte Carlo sweeps here is just $N_E + N_S(n_R + 1)N_M$. One Monte Carlo sweep includes assignments of "deletion" or "freezing" to all bonds and attempts to flip all clusters. The numbers used in our computation are listed in

TABLE I. The parameters used in the computation and the results. The value $K_c = 0.221\,658\,64$ given in [26] was used. All the results presented are obtained through the cluster algorithm except for (a). The figures in parentheses are one-standard-deviation estimates for the statistical errors. The rows (a) and (b) are included only for comparison of the conventional algorithm (a) and the cluster algorithm (b).

L	K	N_S	N_E	N_M	n_R	ξ	g	$(K/K_c)^{3/2}g$
8	0.149 05	7	1000	10 000 000	0	0.800 05(2)	45.38(2)	25.106(11)
16	0.1916	35	2000	200 000	0	1.6024(2)	31.90(14)	25.64(11)
32	0.2108	35	2000	200 000	0	3.2300(5)	27.34(16)	25.36(15)
64	0.2180	28	1000	100 000	0	6.5843(20)	25.47(34)	24.85(33)
(a)16	0.1916	40	70	20 000	6	1.6070(39)	35.5(2.3)	28.5(1.8)
(b)16	0.1916	40	2000	4000	0	1.6033(14)	31.9(9)	25.7(7)

Table I. Since the autocorrelation time is, regardless of the definition, less than 100 [23] up to the system size of 64^3, the numbers N_E and N_M listed in the table are large enough to exclude systematic error due to autocorrelation. As mentioned already, the temperature of the simulation is chosen so that the resulting correlation length becomes approximately $1/10$ of the system size. The actual value of K_c enters our calculations in only a very minor way. Tamayo and Gupta [10] quote 0.221 655, Ferrenberg and Landau [24] quote $0.221\,6595 \pm 26$, and Guttmann [25] using series analysis quotes $0.221\,657 \pm 12$. We have used Rosengren's conjecture [26], $K_c \approx 0.221\,658\,64$. For pseudorandom numbers, we have used the Tausworthe generator.

The results of the simulation are listed in Table I. From the three data for the system with $L = 16$, it is obvious that the present algorithm outperforms the conventional algorithm (single-spin-flip Metropolis algorithm). The advantage of the cluster algorithm is more significant for larger lattices. The results for the 64 cube required about 1100 IBM RS/6000 model 590 h.

In order to assure that we are controlling possible systematic errors, we have performed exact computations on the two cube and the three cube at temperatures which correspond to $\xi = 0.2$ and 0.3, respectively. These results were compared with series expansion results, and we found that the two cube is about 2.2% below and the three cube about 0.8% below the infinite systems series results. In addition, we have compared our very long run, highly accurate Monte Carlo results for the eight cube (Table I) with the series results. We find that it is about 0.2% below the unbiased Padé approximant (see, for example, [9]) estimate. We conclude from these comparisons that it is very likely that the systematic errors are less than 1%, and perhaps much better.

We illustrate our results in Fig. 1. It can be seen that the central extrapolation of Ref. [12] (which we have extended by incorporating two more series terms), which tends to zero, falls well below our present results. We believe that this method does not properly account for the leading subdominate behavior. In [17] it was seen that g^* lies above the limit of $g(K_c, L)$ as $L \to \infty$ in the two-dimensional Ising model. In [10] using the histogram method, it was found that the value of $g(K, L)$ falls very rapidly to 6–7 as $K \to K_c$. Combining these results with ours, we conclude that the value of g^* is greater than zero and so hyperscaling holds for the three-dimensional Ising model. We definitely expect $25 > g^* \gg 6$. We remind the reader of the caution of Nickel [27] who found nonanalytic corrections to the Callan-Symanzik beta function $\beta(g)$ in one dimension, and suggested that there may also be such in other dimensions which would adversely effect the quoted error estimates for the field theory results.

We wish to thank the Advanced Computing Laboratory for making some computer time available to us. This work was supported in part by the U.S. DOE and in part by the University of Tokyo.

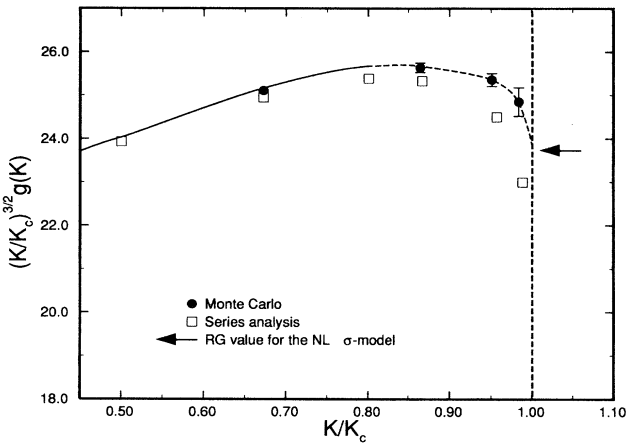

FIG. 1. The renormalized coupling constant [times $(K/K_c)^{1.5}$] vs K/K_c. The solid line represents the series extrapolations as far as their apparent errors are less than the size of our dots. The dashed continuation is drawn in to guide the eye. The symbols ⧫ denote our Monte Carlo results with one-sigma error bars attached. The symbols □ are from the same type of analysis as in the work of Ref. [12]. Cross comparison with other analyses shows that realistic errors on this series extrapolation are sufficiently large so as not to exclude our current Monte Carlo results. The field theoretic renormalization group value is indicated by ←.

*On leave from the Physics Department, University of Tokyo, Tokyo, Japan.
[1] L. P. Kadanoff, Physics **2**, 263 (1966).
[2] G. Stell, Phys. Rev. Lett. **24**, 314 (1970).
[3] M. E. Fisher, in *Collective Properties of Physical Systems,* Proceedings of the Twenty-Fourth Nobel Symposium (Academic, New York, 1970), pp. 16–37.
[4] R. Schrader, Phys. Rev. B **14**, 172 (1976).
[5] G. A. Baker, Jr., and S. Krinsky, J. Math. Phys. (N.Y.) **18**, 590 (1977).
[6] K. G. Wilson, Phys. Rev. B **4**, 3174 (1971); **4**, 3184 (1971).
[7] E. Brézin, J.-C. LeGuillou, and J. Zinn-Justin, Phys. Rev. D **15**, 1544 (1977); **15**, 1558 (1977).
[8] W. J. Camp, in *Phase Transitions, Cargèse 1980,* edited by M. Lévy, J.-C. LeGuillou, and J. Zinn-Justin (Plenum, New York, 1982), pp. 153–267.
[9] G. A. Baker, Jr., *Quantitative Theory of Critical Phenomena* (Academic, Boston, 1990).
[10] P. Tamayo and R. Gupta (to be published). We are grateful for permission to cite this work in advance of publication.
[11] G. A. Baker, Jr., Phys. Rev. B **15**, 1552 (1977).
[12] G. A. Baker, Jr., and John M. Kincaid, J. Stat. Phys. **24**, 469 (1981).
[13] B. A. Freedman and G. A. Baker, Jr., J. Phys. A **15**, L715 (1982).
[14] M. N. Barber, R. B. Pearson, D. Toussaint, and J. L. Richardson, Phys. Rev. B **32**, 1720 (1985).
[15] K. Binder, M. Nauenberg, V. Privman, and A. P. Young, Phys. Rev. B **31**, 1498 (1985).
[16] G. A. Baker, Jr., and J. J. Erpenbeck, *Computer Simulation Studies in Condensed-Matter Physics VII,* edited by D. P. Landau, K. K. Mon, and H.-B. Schuttler, Springer Proceedings in Physics Vol. 78 (Springer, Berlin, 1994), pp. 213–218.
[17] G. A. Baker, Jr., J. Stat. Phys. **77**, 955 (1994).
[18] R.-H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58**, 86 (1987).
[19] For a brief review, see R. H. Swendsen, J.-S. Wang, and A. M. Ferrenberg, in *The Monte Carlo Method in Condensed Matter Physics,* edited by K. Binder (Springer, Berlin, 1991).
[20] N. Ito, Int. J. Mod. Phys. C **5**, 1 (1994).
[21] U. Wolff, Phys. Rev. Lett. **60**, 1461 (1988); Nucl. Phys. **B300 [FS22]**, 501 (1988).
[22] F. Cooper, B. Freedman, and D. Preston, Nucl. Phys. **B210 [FS6]**, 210 (1982).
[23] J.-S. Wang, Physica (Amsterdam) **164A**, 240 (1990).
[24] A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991).
[25] A. J. Guttmann, J. Phys. A **20**, 1855 (1987).
[26] A. Rosengren, J. Phys. A **19**, 1709 (1986).
[27] B. G. Nickel, in *Phase Transitions, Cargèse 1980* (Ref. [8]), pp. 291–324.