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Renormalized coupling constant in the Ising model

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Abstract. The three-dimensional Ising model is studied by means of the Swendsen–Wang, cluster, Monte Carlo method. The simulations are performed on finite sized systems up to the 96-cube, and the renormalized coupling constant is estimated to be $g^* = 25.0(5)$. We make further arguments and computations and say that $g^* \geqslant \hat{g}$ and $4.5 \lesssim \hat{g} \lesssim 5.4$ so that $g^* > 0$ which implies the *validity of hyperscaling*. The Josephson hyperscaling relation also appears to hold. We give estimates for some of the critical indices.

1. Introduction and summary

For about a third of a century there has been uncertainty about a fundamental question in the theory of critical phenomena. The question is whether the 'hyperscaling hypothesis' is valid or not. We will report our results on this question for the three-dimensional Ising model. (A preliminary report was given in [1].) The hyperscaling hypothesis relates to the relations between critical indices which depend on the spatial dimension. To understand what the question really is, we give some background. The Ising model, of course, is defined by spin variables on a spatial lattice which can take on the values ± 1. The Hamiltonian, $\mathcal{H}$, for the model is the exchange energy J times the sum of the products of all the nearest-neighbour spins. We consider the ferromagnetic case where $J > 0$, and abbreviate J/kT to K, where k is Boltzmann's constant and T is the temperature. An important set of objects to study in this model is the set of spin–spin correlations. We define them in terms of $S_A = \prod_{i\in A} s_i$, where the s_i are the individual spins and A is an index set. Then the spin–spin correlations $\langle S_A\rangle$ are the expectation values with respect to the Gibbs weight $\exp(-\mathcal{H}/\|\mathcal{T})/\mathcal{Z}$, where Z is the partition function which is just the normalization for the Gibbs weight. These correlation functions have a number of important properties. Griffiths [2] showed that $\langle S_A\rangle \geqslant 0$, and (generalized by Ginibre [3]) that $\langle S_A S_B\rangle - \langle S_A\rangle\langle S_B\rangle \geqslant 0$. In addition they possess [4] the cluster property, $\langle S_A S_B\rangle - \langle S_A\rangle\langle S_B\rangle \leqslant \mathrm{O}(\mathrm{e}^{-\mu^2\rho})$ where ρ is the distance between A and B and μ is defined by the two-point correlation function through the relation

$$\lim_{r\to\infty}\langle s_{\boldsymbol{s}} s_{\boldsymbol{s}+\boldsymbol{r}}\rangle \propto \exp(-\mu^2|\boldsymbol{r}|). \tag{1.1}$$

In equation (1.1) we consider the case where $K < K_c$, the critical value, as here $\langle s_i\rangle = 0$ and the two-point function decays exponentially [5, 6]. In addition they have the property of 'two-point dominance' as shown by the Lebowitz [7] four-point inequalities,

$$\langle s_i s_j s_k s_l\rangle - \langle s_i s_j\rangle\langle s_k s_l\rangle \leqslant \langle s_i s_k\rangle\langle s_j s_l\rangle + \langle s_i s_l\rangle\langle s_j s_k\rangle \tag{1.2}$$

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and for higher-point correlations by Newman's [8] Gaussian inequalities. These are unusual inequalities in the sense that higher-point expectation values are bounded in terms of lower-order ones. In equation (1.2), if spins i and j are close together but far from l and k, we have an example of the cluster property. To get ahead of the story, the key question turns out to be whether the inequalities like (1.2) saturate and become equalities or not.

To be more quantitative, let us define a few quantities. First the magnetic susceptibility is given by

$$\chi(K, L) = L^{-d} \sum_{i,j} \langle s_i s_j \rangle \tag{1.3}$$

where for ease of exposition we consider the hyper-cubic lattice family with edge L in spatial dimension d. The critical point K_c is the smallest value of K for which χ diverges. It is at this point that the μ defined above goes to zero. It is convenient to define the correlation length, ξ which is related to μ^{-2}:

$$\xi^2(K, L) = \frac{\sum_{\boldsymbol{r},\boldsymbol{s}} |\boldsymbol{r}|^2 \langle s_{\boldsymbol{s}} s_{\boldsymbol{s}+\boldsymbol{r}} \rangle}{2dL^d \chi} \tag{1.4}$$

and also to define the second derivative of χ with respect to the magnetic field H as

$$\frac{\partial^2 \chi}{\partial H^2} = L^{-d} \sum_{\boldsymbol{r},\boldsymbol{s},\boldsymbol{t},\boldsymbol{u}} [\langle s_{\boldsymbol{r}} s_{\boldsymbol{s}} s_{\boldsymbol{t}} s_{\boldsymbol{u}} \rangle - \langle s_{\boldsymbol{r}} s_{\boldsymbol{s}} \rangle \langle s_{\boldsymbol{t}} s_{\boldsymbol{u}} \rangle - \langle s_{\boldsymbol{r}} s_{\boldsymbol{t}} \rangle \langle s_{\boldsymbol{s}} s_{\boldsymbol{u}} \rangle - \langle s_{\boldsymbol{r}} s_{\boldsymbol{u}} \rangle \langle s_{\boldsymbol{s}} s_{\boldsymbol{t}} \rangle]\,. \tag{1.5}$$

All of these quantities diverge at the critical point as some power of $(K_c - K)$. The conventional notation is

$$\chi \propto (K_c - K)^{-\gamma} \qquad \xi \propto (K_c - K)^{-\nu} \qquad \frac{\partial^2 \chi}{\partial H^2} \propto (K_c - K)^{-\gamma - 2\Delta} \tag{1.6}$$

which defines the critical exponents or indices γ, ν, and Δ. It is known [9, 10] that these critical indices satisfy the inequality

$$\gamma + \mathrm{d}\nu \geqslant 2\Delta. \tag{1.7}$$

If we take the idea [11, 12] that there is only one important length near the critical point and that it is ξ, and that everything is a function of the ratio of the distances to ξ, then we come to the conclusion that we should have an equality

$$\gamma + \mathrm{d}\nu = 2\Delta \tag{1.8}$$

which is a *hyperscaling relation*. This equality is equivalent to the idea that the cluster property holds with a non-zero coefficient for the four-point, spin–spin correlation function, no matter how we pair up the variables. At this point it is worthwhile remembering a feature of the Gaussian model. (This model is the same as the Ising model, except that instead of the spin variables taking on only the values ± 1, all real values are taken with probability $\mathrm{e}^{-s^2/2} ds/\sqrt{2\pi}$.) In this model, the $\leqslant$ sign becomes a $\equiv$ sign in (1.2) and $\partial^2\chi/\partial H^2 \equiv 0$. This result shows that there is, in principal, no restriction on reasonable models that prevents the leading order of the correlation functions from cancelling out. When this cancellation occurs, the inequality sign is the correct one, and the hyperscaling hypothesis fails. Aizenman [13] has shown that it also fails for the Ising model for $d > 4$. On the other hand, for the two-dimensional Ising model the hyperscaling hypothesis is valid [13, 14]. For the one-dimensional Ising model, equation (1.8), as appropriately modified to take account of the zero-temperature critical point, holds [15].

We mention that there is another hyperscaling relation involving the specific heat index α which converts the Josephson inequality [16], $\mathrm{d}\nu \geqslant 2 - \alpha$ into an equality. The index

α is defined by $C_H \propto (K_c - K)^{-\alpha}$ in the limit as $K \to K_c$. This relation fails [15] in one-dimension, and can at best be said to hold weakly in two-dimensions, because in two-dimensions $\nu = 1$ and the specific heat at constant magnetic field C_H diverges as $\ln(K_c - K)$ which corresponds to an α of zero. All of these exponent relations correspond to the critical point limit of the logarithm of estimator functions. If instead we look at the estimator function, we expect it to approach a finite number at the critical point when hyperscaling holds. In the case of a logarithmic approach, this expectation is not fulfilled, and the estimator function fails to satisfy the expected properties, but does not, strictly speaking, cause a failure in the exponent relations. In three-dimensions, our data is consistent with the validity of this hyperscaling relation.

The interest in this question for $d = 3, 4$ was heightened with the introduction of the renormalization group theory of critical phenomena by Wilson [17], for which he won the 1982 Nobel prize in physics. One of the most powerful computational tools for this theory is the field theory method with its expansion in variable dimension, i.e. the ϵ-expansion [18]. The hyperscaling hypothesis is implicitly assumed in the method and it would be a matter of extreme importance if it should fail, as it would have a deleterious effect on a very large number of computations which have been carried out using this method, not to mention the problem of a proper understanding of the physics which would be associated with such a failure.

A quantitative way to examine this question is by an examination of the 'renormalized coupling constant', g^*. First we define the estimator function,

$$g(K, L) = -\left(\frac{v}{a^d}\right) \frac{\partial^2 \chi}{\partial H^2} \bigg/ \chi^2 \xi^d \tag{1.9}$$

from which the renormalized coupling constant is defined by

$$g^* = \lim_{K \to K_c - 0} \lim_{L \to \infty} g(K, L). \tag{1.10}$$

It follows from equation (1.7) that g^* does not diverge to infinity. If $g^* > 0$, then the hyperscaling relation (1.8) holds. If $g^* = 0$, then hyperscaling may fail. Hara and Tasaki [19] have proved in four dimensions that $g(K, \infty) \propto [n_0 + |\ln(K_c - K)|]^{-1/2}$ which means that $g^* = 0$. However, it vanishes logarithmically, so equation (1.8) holds, but only weakly. The remaining case is for $d = 3$, which is what we will investigate in this paper. In the field theory approach the renormalized coupling constant is estimated [20] as $g^* \approx 23.73(2)$.

In his 1967 review, Fisher [21] fully summed up the then current status of the hyperscaling relations as, 'These relations involving the dimensionality directly seem most open to question, ...'. In a subsequent series analysis Baker [22] estimated that $2\Delta - d\nu - \gamma \equiv -\omega^* \approx -0.028$. It is this type of counter-hypothesis that has made this issue so difficult to resolve. It says that perhaps $g(K, \infty)$ vanishes as $K \to \infty$, but as a very small power of $(K_c - K)$. Practically speaking, in this case, the curve should show almost no deviation from one which tends to a constant limit until one is very close to the critical point, and then it drops precipitously. Thus direct computation of the $g(K, \infty)$ or $g(K, L)$ as $K \to K_c$, considering the practical limitations of such calculations, cannot really demonstrate the validity of hyperscaling. In this paper, we take a two-pronged approach to the resolution of this issue. First, we compute $g(K, L)$ directly by a Monte Carlo procedure for a sequence of system sizes so that we keep ξ/L fixed. We will argue that we have chosen a small enough value to keep systematic errors at, or below, the 1% level. This method will provide a direct estimate of g^*, provided $\omega^* = 0$ without logarithmic corrections.

The point $K = K_c$, $L = \infty$ is a very special point. We will show, when we are very specific about the definition of our estimator $g(K, L)$, that the limit from the low-temperature side,

$$g^{\ddagger} = \lim_{K \to K_c + 0} \lim_{L \to \infty} g(K, L) = 0 \tag{1.11}$$

if hyperscaling is valid, is not equal to g^*. Thus this point is what is called a point of non-uniform approach. We will argue that the limit

$$\hat{g} = \lim_{L \to \infty} \lim_{K \to K_c} g(K, L) \tag{1.12}$$

is a lower bound to g^* and our calculations show that $\hat{g}$ is distinctly greater than zero, and so $g^* > 0$, which in turn implies that the hyperscaling relation (1.8) is valid, which was our main point of inquiry. Note that the quantity $g^{\ddagger}$ is not the same as the renormalized coupling constant g_-^* that is computed from a proper approach to the critical point from the low temperature side, nor is it the ratio of the corresponding, critical-point amplitudes G_1^- taken on the low-temperature side. These latter quantities are discussed by Zinn *et al* [23].

To our knowledge, the first clear illustration of the fact that $K = K_c$, $L = \infty$ is a point of non-uniform approach for $g(K, L)$ is that given by Baker [24] from exact calculations by the Markov property method for small two-dimensional squares with periodic boundary conditions. We reproduce his figure here as figure 1. In this figure we see for $K < K_c$ that the finite size system results are approaching the infinite system size limit in a straightforward fashion. However, for $K = K_c$, the values of $g(K_c, L)$ seem instead to be approaching a limit around 3 instead of the value of $g^* \approx 14.66 \pm 0.06$. It is this result which foreshadowed the present work.

From the practical point of view, another important insight was the recognition of Baker and Erpenbeck [25] of the data collapse which results from plotting the renormalized coupling $g(K, L)$ versus ξ_L/L (see also Kim and Landau [26]). The same data collapse does not occur if the plot is made of $g(K, L)$ versus ξ_∞/L, for example. We reproduce Baker and Erpenbeck's figure here as figure 2. In addition these authors report a clear warning that care must be taken not to use too large a value of ξ_L/L. They demonstrate that $\xi_L/L = 0.26$ is too large for accurate work, which means that some of the prior efforts in the investigation of this area would be likely to suffer from significant systematic errors. Baker [24] had observed that for the two-dimensional systems he found that $\xi_L/L \leqslant 1/(7 \pm 1)$ was required for 1% accuracy. Baker and Erpenbeck further observed that the allowed value of ξ_L/L for, say, 1% accuracy seems to increase somewhat with L and concluded that for large systems the maximum allowed value of ξ_L/L must be somewhere in the range 0.11–0.26. They recommended that $\xi_L/L \leqslant 0.10$ for work at 1% accuracy.

In the second section we describe our Monte Carlo method, which is a cluster method. Our main contribution here is the introduction of improved estimators for the second partial derivative of the susceptibility with respect to the magnetic field and for the wavevector-dependent susceptibility. It is mainly this improvement in the estimators that has made it feasible to do all our computations. In the third section we report our Monte Carlo results and use them to give our direct estimate of $g^* \approx 25.0 \pm 0.5$. We have computed results for a series of cubes of increasing size for temperatures which correspond to $\xi_L/L \approx 0.1$. Our largest system size is the 96-cube for which it took of the order of 20 processor months to perform the required computations. In section 4 we show that $g^{\ddagger} = 0$ for the estimators we are using. In section 5 we discuss the value of $4.5 \lesssim \hat{g} \lesssim 5.4$. That $\hat{g} > 0$ is crucial to the argument that hyperscaling holds, and we find this result to be true by a wide margin with respect to our error estimates. In section 6, we discuss briefly the Josephson hyperscaling relation, $d\nu = 2 - \alpha$. Our evidence is consistent with the hypothesis that this relation also holds. Finally, in section 7 we use our Monte Carlo results to estimate some of the critical indices. We conclude that these estimates agree within errors with those predicted by the

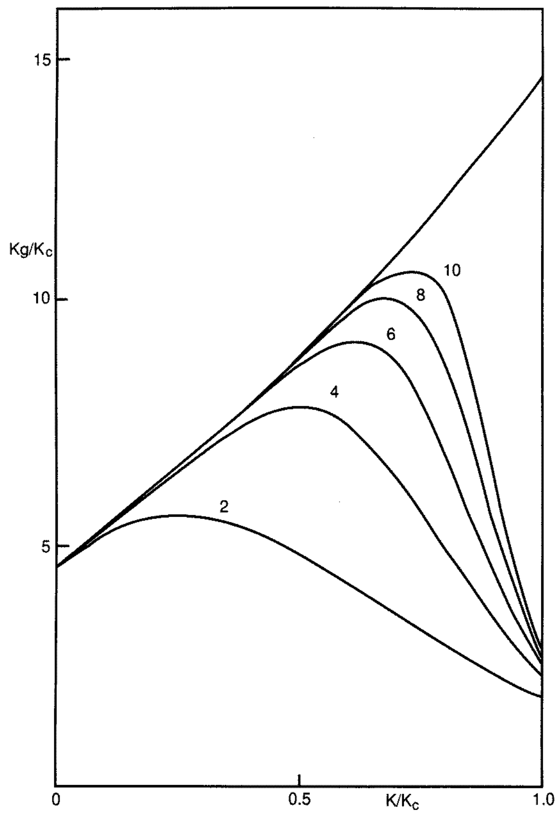


Figure 1. A plot of $Kg(K, L)/K_c$ versus K/K_c for the two-dimensional Ising model. The unlabelled curve is the series result for an infinite system, and the labels L indicate the curves for $L \times L$ square lattices with periodic boundary conditions.

renormalization group, except for the specific-heat index, which we believe we have not estimated in a reliable manner.

2. Method of calculation

In our computations a Monte Carlo method was employed. For pseudo-random numbers, we employed the Tausworthe generator. We used the Swendsen–Wang algorithm [27] for spin updating. This type of algorithm has two advantages over the conventional algorithm, namely reduction in the autocorrelation time, and reduction in the variances of equilibrium distributions of relevant quantities. As has been reported by several authors [28], we observed that the cluster algorithm with improved estimators dramatically reduces statistical errors. It was reported [29] that cluster algorithms are not necessarily much more efficient than conventional algorithms with multi-spin coding techniques when only the first benefit, i.e. the reduction in the correlation time, 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 those presented in [1] by means of a conventional algorithm within a reasonable computation time ($\sim$ a few months) and within

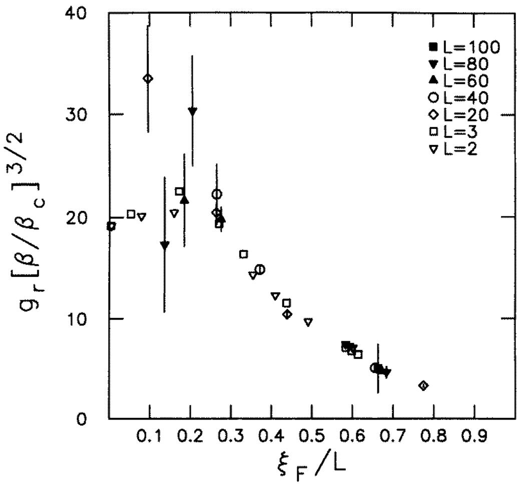


Figure 2. A plot of $g(K, L)(K/K_c)^{3/2}$ for the three-dimensional Ising model for the simple cubic lattice with periodic boundary conditions. The cases shown are for systems of $L \times L \times L$ spins, and the plot is versus ξ_L/L. The point $\xi_L = 0$ is common for all values of L and is exact.

the given resources, at the temperatures of the present interest. Our present computations were performed on a cluster of eight IBM RS/6000 model 590's, SUN 5's, UltraSparcs, a SparcServer2000, a Sun20, a Power PC and a PC pentium 90. As we will show, even for smaller lattices it was obvious that the cluster algorithm performs better.

It is known [30] that a Monte Carlo simulation with a cluster algorithm, such as the one used in this paper, can be viewed as a Markov process in an extended configuration space that is a product of the original spin-configuration space and a graph space. Various physical quantities defined in terms of spin variables have corresponding definitions in graphical terms as well. For instance, it is well known that we can estimate the susceptibility, which is usually defined as the second moment of the total magnetization, as the average volume of clusters. It is also known that the equilibrium distribution functions of two corresponding estimators, one in terms of spins and the other in terms of graphs, can have very different variances although the mean values are equal. In the above example, the graphical estimator is more advantageous because it has a much smaller variance than the estimator defined on spin configurations.

Since we will deal with the renormalized coupling constant, which is a product of several macroscopic quantities, we need to obtain the graphical representation of all the quantities involved. Otherwise the relative error associated with the quantity estimated through the poor estimator would be much larger than the relative errors from other sources and it would dominate the relative error in the final estimate. First we rewrite the definition of the renormalized coupling constant equation (1.9) as

$$g(K, L) \equiv -\left(\frac{L}{\xi_L}\right)^d \frac{\langle M^4\rangle - 3\langle M^2\rangle^2}{\langle M^2\rangle^2}. \tag{2.1}$$

Therefore, we need improved estimators for ξ_L, $\langle M^2\rangle$ and $\langle M^4\rangle$.

A new graphical estimator for the correlation length ξ_L is derived as follows. We define

$$f(\boldsymbol{k}) \equiv 4\left(\sin^2\frac{k_x}{2} + \sin^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\right)\left(1 - \frac{\chi(\boldsymbol{k})}{\chi}\right)^{-1} \tag{2.2}$$

with

$$\chi(\boldsymbol{k}) \equiv \langle |M(\boldsymbol{k})|^2 \rangle / N \tag{2.3}$$

where $M(\boldsymbol{k}) = \sum_{\boldsymbol{r}} \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) S_{\boldsymbol{r}}$. The quantity $f(\boldsymbol{k})$ converges to ξ_L^{-2} in the limit of $L \to \infty$ and $|k| \to 0$ with a correction term proportional to $|k|^2$. In order to eliminate this correction term, we formed a linear combination of $f(\boldsymbol{k})$ with six smallest possible values of $|\boldsymbol{k}|$ which correspond to the nearest and the second-nearest neighbours to the origin in the reciprocal space:

$$\begin{aligned}\xi_L^{-2} = [&2f(\Delta k, 0, 0) + 2f(0, \Delta k, 0) + 2f(0, 0, \Delta k) - f(0, \Delta k, \Delta k) \\ &- f(\Delta k, 0, \Delta k) - f(\Delta k, \Delta k, 0)]/3\end{aligned} \tag{2.4}$$

where $\Delta k \equiv 2\pi/L$. This expression is correct up to the second order in $1/L$ and we estimated ξ_L through it. Thus estimation of ξ_L is reduced to computing $\langle |M(\boldsymbol{k})|^2 \rangle$ for several smallest reciprocal vectors.

It is well known that an improved estimator for the second moment of magnetization is simply the average size of clusters [31], i.e.

$$\langle M^2 \rangle = \left\langle \sum_c V_c^2 \right\rangle. \tag{2.5}$$

Here, V_c is the number of sites in a cluster c. For the fourth moment of magnetization, we can derive by the same methods the corresponding estimator,

$$\langle M^4 \rangle = 3\left\langle \left(\sum_c V_c^2 \right)^2 \right\rangle - 2\left\langle \sum_c V_c^4 \right\rangle. \tag{2.6}$$

We can express $\chi(\boldsymbol{k})$ in a form analogous to equation (2.5):

$$\langle M^2(\boldsymbol{k}) \rangle = \left\langle \sum_c V_c(\boldsymbol{k})^2 \right\rangle \tag{2.7}$$

with

$$V_c(\boldsymbol{k}) \equiv \left| \sum_{\boldsymbol{r}\in c} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) \right|. \tag{2.8}$$

Thus, we have expressed all the necessary quantities in terms of improved estimators.

Our simulation consists of N_{S} independent runs. Each run consists of N_{E} sweeps for equilibration followed by $N_{\mathrm{M}}(1 + n_{\mathrm{R}})$ Monte Carlo sweeps for measurement. Actual measurements are done every $(1+n_{\mathrm{R}})$ steps and therefore the number of total measurements performed in each run is N_{M}. Accordingly, the total number of Monte Carlo sweeps performed in the whole simulation is $N_{\mathrm{total}} \equiv N_{\mathrm{S}}[N_{\mathrm{E}} + (n_{\mathrm{R}} + 1)N_{\mathrm{M}}]$. (The item marked by '*a*' in table 1 was performed in a different fashion from this. For this simulation, the equilibration sweeps were not for the second or later runs, but only at the beginning of the whole simulation. Therefore, N_{E} in table 1 for the item refers only to the first run, so the total number of Monte Carlo sweeps here is just $N_{\mathrm{E}} + N_{\mathrm{S}}(n_{\mathrm{R}} + 1)N_{\mathrm{M}}$.) In the conventional algorithm is it necessary to take $n_{\mathrm{R}} > 0$. 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 1. Since the autocorrelation time is, regardless of the definition, less than 100 [32] up to the system size of 96^3, the numbers N_{E} and N_{M} listed in the table are large enough to exclude systematic errors due to autocorrelation. As mentioned already, the temperature of the simulation is chosen so that the resulting correlation length becomes approximately $\frac{1}{10}$ of the system size. We used the value of K_c in multiplying the estimate $g(K)$ by the factor $(K/K_c)^{3/2}$. Adding this factor is appropriate

Table 1. The parameters used in the computation, and the results.

	L	K	N_S	N_E	N_M	n_R	N_{total}	ξ	Δ
	8	0.149 05	7	1000	1×10^7	0	7.0×10^7	0.800 05(2)	0.011
	16	0.1916	35	2000	2×10^5	0	7.1×10^6	1.6024(2)	0.11
	32	0.2108	35	2000	2×10^5	0	7.1×10^6	3.2300(5)	0.15
	64	0.2180	28	1000	1×10^5	0	2.8×10^6	6.5843(20)	0.33
	96	0.2197	41	1000	7×10^4	0	2.9×10^6	9.8309(31)	0.32
a	16	0.1916	40	70	2×10^4	6	5.6×10^6	1.6070(39)	1.8
b	16	0.1916	40	2000	4×10^3	0	2.4×10^5	1.6033(14)	0.7

The value $K_c = 0.221\,6546$ given in [36] was used. All the results presented are obtained through the cluster algorithm except for a. The last column Δ is the estimated statistical error in $(K/K_c)^{3/2} g(K, L)$. The rows a and b are included only for comparison of the conventional algorithm (a) and the cluster algorithm (b).

because the quantity $g(K)$ has for small K the dependence $g(K) \propto K^{-3/2}$. As the actual value of K_c, we can use almost any one of very accurate estimates available today, and the choice does not affect the present result in any significant way. For example, Gupta and Tamayo [33] quote 0.221 655, Ferrenberg and Landau [34] quote $0.221\,6595 \pm 26$ and Guttmann [35] using series analysis quotes $0.221\,657 \pm 12$. We used Blöte *et al*'s value $K_c = 0.221\,6546(10)$ [36]. This latter quoted error makes a difference of at most 0.05% in $K_c - K$ in our cases.

3. Results for the direct estimation of g^*

In order to estimate g^*, we choose for each system size L the temperature T so that L/ξ is fixed to be a constant R. In the present paper we take $R = 10$ for various reasons mentioned in the first section. In other words, we estimated $g(K, R\xi(K))$ in practice. In order to ensure that we are controlling possible systematic errors, we have performed exact computations on the 2-cube and the 3-cube at temperatures which correspond to $\xi_L = 0.2$ and 0.3 respectively. These results were compared with series expansion results, which yield very precise estimates for $g(K, \infty)$ in such a temperature range, and we found that the 2-cube result is about 2.2% below and the 3-cube one 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 8-cube, table 1, with the series results. We find that it is about 0.2% below the unbiased Padé approximant (see, for example, [37]) estimate. We conclude from these comparisons that it is very likely that the systematic errors $|g(K, R\xi(K)) - g(K, \infty)|$ are less than 1%, and perhaps much less.

We have obtained results for $g(K, R\xi(K))$ for a sequence of temperatures with

Table 2. The estimates for various quantities.

L	$\langle M^2 \rangle$	$\langle M^4 \rangle - 3\langle M^2 \rangle^2$	$\langle E^2 \rangle - \langle E \rangle^2$	g	$(K/K_c)^{3/2} g$	$\langle E \rangle$
8	$4.207\,00(7) \times 10^0$	$-4.113(2) \times 10^2$	4.1554(6)	45.38(2)	25.02(1)	−0.494 377(8)
16	$1.2776(2) \times 10^1$	$-2.143(9) \times 10^4$	6.092(4)	31.9(1)	25.6(1)	−0.703 30(2)
32	$4.5681(8) \times 10^1$	$-1.92(1) \times 10^6$	9.224(7)	27.3(2)	25.4(2)	−0.843 83(1)
64	$1.7752(6) \times 10^2$	$-2.29(3) \times 10^8$	13.55(2)	25.5(3)	24.9(3)	−0.922 51(1)
96	$3.860(1) \times 10^2$	$-3.61(5) \times 10^9$	16.45(2)	25.5(3)	25.2(3)	−0.947 670(6)

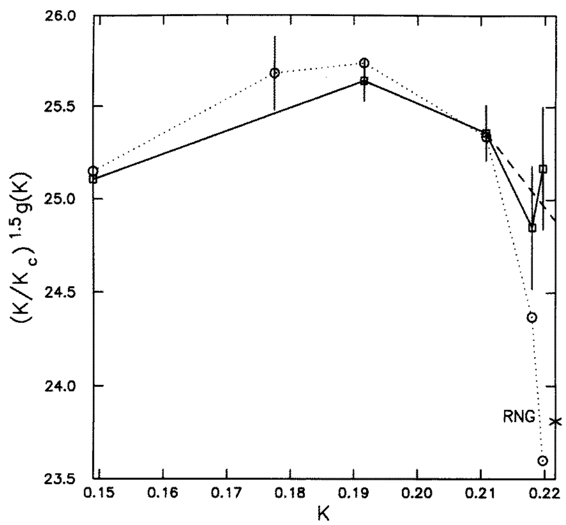


Figure 3. The renormalized coupling constant $g(K, L)$ times $(K/K_c)^{3/2}$ versus K/K_c. The open squares correspond to the simulations for $L = 8, 16, 32, 64$ and 96, from the left to the right, respectively. The dotted curve is merely to guide the eye. The error bars represent one standard deviation. The series analysis results are from the same type of analysis as in the work of [38] and are marked by the open circles. The apparent errors are not displayed here for $K > 0.19$ to avoid clutter. At the temperature of the 16-cube point the error is about ± 0.4 and it is about ± 3 for the rest of the points. The field-theoretic, renormalization-group value is indicated at the right margin of the figure.

$R = L/\xi \approx 10$ for various temperatures. The parameters used in simulations are listed in table 1. We tabulate our results in table 2, and illustrate some of them in figure 3. We conclude that $g^* = 25.0(5)$. It can be seen that the central extrapolation of [38], which tends to zero, falls well below our present results. We believe that this method does not properly account for the leading subdominate behaviour. However, at the temperature of the 8-cube point, it agrees with the unbiased Padé approximant mentioned above in that the Monte Carlo result is about 0.2% lower. We take note that these series results were wrongly plotted in our preliminary report [1]. We remind the reader of the caution of Nickel [39] who found non-analytic corrections to the Callan–Symanzik beta function $\beta(g)$ in one-dimension, and suggested that there may also be such corrections in other dimensions which would adversely effect the quoted error estimates for the field theory results, $g^* \approx 23.73(2)$. In [24] 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 [33] using the histogram method, it was found that the value of $g(K, L)$ falls very rapidly to about 5 as $K \to K_c$. Combining these results with ours, we will conclude in the next two sections that the value of g^* is greater than zero and so hyperscaling holds for the three-dimensional Ising model.

4. Value of $g^\ddagger$

In this section we discuss $g^\ddagger$ as defined by equation (1.11). Our starting point is the definition of $g(K, L)$ given by equation (2.1). If we sum the Lebowitz inequality (1.2) over all values of the lattice sites for each of the four subscripts, then we see that the numerator of the second factor is necessarily non-positive which means, by the positivity of the separate terms and Griffith's second inequality that

$$2 \geqslant \frac{3\langle M^2\rangle^2 - \langle M^4\rangle}{\langle M^2\rangle^2} \geqslant 0, \tag{4.1}$$

and hence it is bounded for all temperatures.

The next quantity to consider is ξ_L/L which is given in our work by equations (2.2)–(2.4). First we need to study the order of magnitude of $\chi(K, \boldsymbol{k})$ for $K > K_c$ and $|\boldsymbol{k}|L = \mathrm{O}(1)$. Let us pick a definite K. This corresponds to a definite spontaneous magnetization m. For a given $\epsilon > 0$ there exists an L such that

$$|\langle\sigma_{\mathbf{o}}\sigma_{\boldsymbol{r}}\rangle - m^2 - g(\boldsymbol{r})| < m^2\epsilon \tag{4.2}$$

uniformly in $\boldsymbol{r}$ for all $\boldsymbol{r}$ in our $L \times L \times L$ cube, where $g(\boldsymbol{r})$ is the two-point correlation function in the thermodynamic limit, which decays (exponentially) towards zero as $|\boldsymbol{r}|$ gets large. We take $\mathbf{0}$ in the centre of the cube for ease of exposition. Since $g(\boldsymbol{r}) \geqslant 0$ by Griffith's second inequality, and for all $K > K_c$ the low-temperature susceptibility, χ_-, is finite by low-temperature series results, and because the spin–spin correlation functions can be proved to converge as the system size goes to infinity, we have the result quoted in the above equation, with $\sum_{\boldsymbol{r}} g(\boldsymbol{r}) = \chi_-$. Near the origin, $g(\boldsymbol{r})$ is necessarily bounded as $|\sigma| = 1$ for the Ising model. Thus for $|\boldsymbol{k}| > 0$

$$\sum_{\boldsymbol{r}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\langle\sigma_{\mathrm{O}}\sigma_{\boldsymbol{r}}\rangle = \sum_{\boldsymbol{r}} \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})g(\boldsymbol{r}) + \mathrm{O}(m^2\epsilon L^d) = \chi_-(K, \boldsymbol{k}) + \mathrm{O}(m^2\epsilon L^d) \tag{4.3}$$

where $\chi_-(K, \boldsymbol{k})$ is a definite quantity, finite-valued, independent of L, and depending only on K and $\boldsymbol{k}$. The only property of $\boldsymbol{k}$ that is used is its orthogonality to the magnetization. In fact as we choose the smallest non-zero, Fourier component for $\boldsymbol{k}$, and by using the strong (i.e. integrable) decay of $g(\boldsymbol{r})$, we might as well substitute $\boldsymbol{k} = \mathbf{0}$ in the sum, which therefore yields just χ_-. Hence, by (2.2),

$$\begin{aligned} L^2 f(\boldsymbol{k}) &= 4L^2\left(\sin^2\frac{k_x}{2} + \sin^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\right)\left[1 - \frac{\sum_{\boldsymbol{m},\boldsymbol{n}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{n}}\langle\sigma_{\boldsymbol{m}}\sigma_{\boldsymbol{n}+\boldsymbol{m}}\rangle}{\sum_{\boldsymbol{m},\boldsymbol{n}}\langle\sigma_{\boldsymbol{m}}\sigma_{\boldsymbol{n}+\boldsymbol{m}}\rangle}\right]^{-1} \\ &= 4L^2\left(\sin^2\frac{k_x}{2} + \sin^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\right) \\ &\quad\times \mathrm{O}\left(\left[1 - \frac{\chi_-(K, \mathbf{0})L^d + \mathrm{O}(m^2\epsilon L^{2d})}{m^2L^{2d} + \chi_-(K, \mathbf{0})L^d}\right]^{-1}\right) \\ &\to 4L^2\left(\sin^2\frac{k_x}{2} + \sin^2\frac{k_y}{2} + \sin^2\frac{k_z}{2}\right)[1 + \mathrm{O}(\epsilon)] \qquad \text{as } L \to \infty. \end{aligned} \tag{4.4}$$

Since ϵ can be taken as small as we please, and since by (2.4) the 1's cancel, we conclude that for any $K > K_c$, and for our estimator for the correlation length, $(L/\xi_L)^d \to 0$ and thus the conclusion which we have already stated in equation (1.11), that $g^\ddagger = 0$, follows.

This conclusion, together with the results of series analysis [37], and both our results and those of others, strongly suggests the conjecture that in the three-dimensional, spin-$\frac{1}{2}$ Ising model for fixed L, $g(K, L)$ is a decreasing function of K. (Baker and Kincaid [38] provide some evidence that this conclusion may not always be valid for the continuous-spin Ising model.) On the basis of this conjecture we can easily write

$$g(K - \delta K, L) \geqslant g(K_c, L) \geqslant g(K + \delta K, L). \tag{4.5}$$

By first taking the limit as $L \to \infty$ of this series of inequalities and then the limit $\delta K \to 0$, we obtain, in the notation of equations (1.10)–(1.12),

$$g^* \geqslant \hat{g} \geqslant g^\ddagger. \tag{4.6}$$

Since $g^{\ddagger} = 0$, as we have just seen, and since we are trying to see if we can determine whether or not $g^* > 0$, which would establish the validity of hyper-scaling, we next turn our attention to $\hat{g}$.

5. The estimation of $\hat{g}$

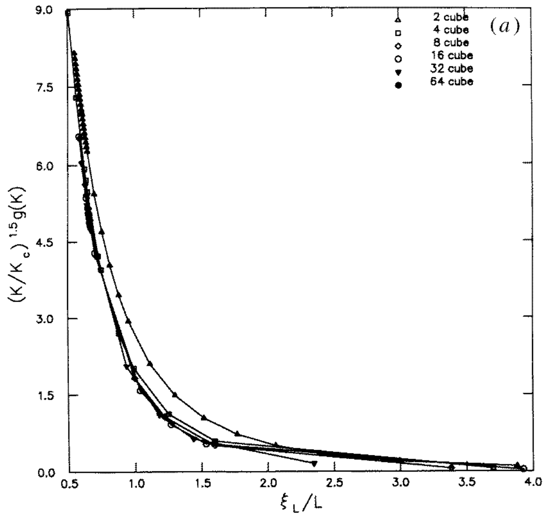
In this section we will focus on the behaviour of the various estimator functions very near the critical point. We have used our Monte Carlo method to compute, for values of K on both sides of the critical value, $g(K, L)$ and $\xi(K, L)$. We have used 300 000–500 000 Monte Carlo sweeps to gather this data. To simulate the histogram method, we have used K-independent random numbers. The smaller number of sweeps was used for the smaller sizes of cubes and the larger number of sweeps for the largest cube. The 2-cube was done exactly. We display them in figure 4, in a manner corresponding to figure 2. The whole range of K reflected in this figure vanishes as $L \to \infty$. This feature is, as we will see, a consequence of the result that $g^* > g^{\ddagger}$ and that the curves for finite L are continuous. Note is also taken that this figure also supports the conclusion of the previous section, namely that $g^{\ddagger} = 0$. We see in this figure that in the region very near the critical point the data collapses rapidly as the system size increases to give a single curve. Thus without going to very large systems, we obtain the profile of g versus ξ_L/L with much less computational effort. We conclude from this figure that the location of the value of $\xi(K_c, L)/L$ and $g(K_c, \infty)$ are for our purposes of finding out whether $\hat{g} > 0$ or not, just two sides of the same coin. Preliminary reports of this part of the work have been made [40, 41].

The simplest method to estimate this quantity was used in [40]. Here all the best current estimates of the critical point (see above) were noted and the results for $g(K, L)$ were computed for this range of K's and a variety of values of L. Their results are displayed in figure 5. It will be seen that this analysis leads to the idea that $\hat{g} = 5.0(3)$.

A more sophisticated approach was used in [41]. The point is that the limit at any point $K \neq K_c$ as the system size tends to infinity will be g^* or $g^{\ddagger}$, so we need to contract the interval in K over which we examine $g(K, L)$ as the system size increases. To this end, it is useful to be able to estimate the uncertainty in the location of the critical point for each value of L. We use two related estimators. The first is due to Binder [42]. He pointed out that the cumulant ratio,

$$U = \frac{\langle M^4 \rangle}{(\langle M^2 \rangle)^2} - 3 \tag{5.1}$$

definitely converges to zero as $L \to \infty$ for $K < K_c$ and to -2 for $K > K_c$. He then argued that it goes to a fixed-point value U_c at $K = K_c$, and so with certain monotonic convergence assumptions he concluded that the $U(K, L)$'s for successive values of L cross at a point which rapidly approaches the critical point. Baker [24] found that, at least for small values of L, this is true in the two-dimensional Ising model and the accuracy of this estimate is about an order of magnitude better than that using the peak in the specific heat. From the picture we have built up of the function $g(K, L)$ the same features should appear for it as did for U. Thus we take the crossing points of $g(K, L)$ for successive values of L as our second estimator. These results are summarized in table 3. It should be noted that values of K for which the crossings of U occur are numerically monotonically decreasing with increasing L, and those for which the crossings of g occur are numerically monotonically increasing. In line with figure 4, the values of g at these latter crossings are monotonically decreasing and may provide an upper bound to $\hat{g}$. Furthermore, within the reported error, all the g crossings are for smaller values of K than for any of the U crossings. Remembering



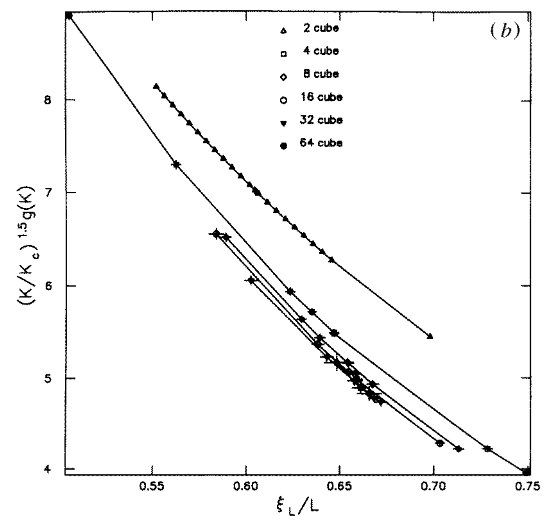


Figure 4. A plot of $g(K, L)(K/K_c)^{3/2}$ for the three-dimensional Ising model for the simple cubic lattice with periodic boundary conditions. The cases shown are for systems of $L \times L \times L$ spins, and the plot is versus ξ_L/L. (*a*) shows a large range of ξ_L/L and (*b*) shows a magnified portion near the critical point. The error bars are one standard deviation, but they mainly do not show in (*a*) because they are inside the 'dots.'

the monotonicity of $g(K, L)$ for fixed L which we discussed previously, we have also tabulated the values of g at the U crossings. This sequence is not as smooth as it might be, but it is mostly monotonically increasing in L. This sequence may form a lower bound to $\hat{g}$. It is reported in [41] that $g(0.221\,655, 64) \approx 4.89(6)$ (they used 400 000 Monte Carlo sweeps). Taking all these results together, at the two-standard-deviation level, we estimate that $4.5 \lesssim \hat{g} \lesssim 5.4$. In terms of (4.6), these results are sufficient to establish $g^* > 0$, which in turn, we think, establishes beyond reasonable doubt the *validity of hyperscaling* for the three-dimensional Ising model!

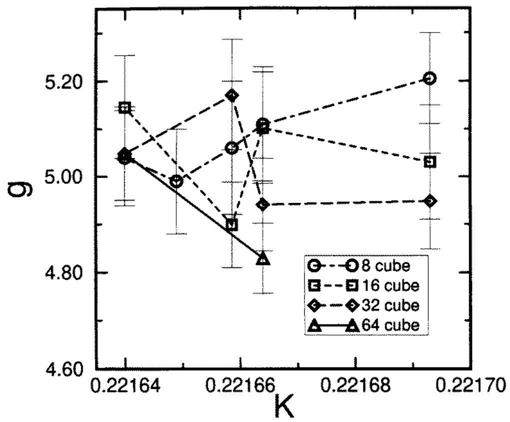


Figure 5. The renormalized coupling constant in the neighbourhood of the critical temperature for several lattice sizes.

Table 3. The curve crossing values of K and g for the curves g and U.

$n \otimes 2n$	$K_{g,\otimes}$	$g_{\otimes}$	$K_{U,\otimes}$	$U_{\otimes}$	$g(K_{U,\otimes}, L)$
$2 \otimes 4$	0.2135(2)	8.24(3)	0.2274(3)	−1.5836(7)	3.96(11)
$4 \otimes 8$	0.2209(1)	5.77(6)	0.2227(1)	−1.501(4)	4.40(11)
$8 \otimes 16$	0.221 56(7)	5.2(1)	0.222 01(2)	−1.489(2)	4.26(7)
$16 \otimes 32$	0.221 64(2)	5.1(1)	0.221 68(2)	−1.425(9)	4.8(2)
$32 \otimes 64$	0.221 65(1)	5.0(2)	0.221 66(1)	−1.414(7)	4.9(2)

6. The hyperscaling relation d$\nu = 2 - \alpha$

We have not made a detailed study of the Josephson, hyperscaling relation d$\nu = 2 - \alpha$ but our results, as reported in tables 1 and 2, do shed some light on its validity. Since the reported errors of the value of K_c are so small as to be relatively unimportant at the distance from the critical-point at which our data is taken, we feel justified in using the biased (by the knowledge of the critical-point location) estimator function,

$$\kappa(K, L) = [(K_c - K)^2 C_H(K, L)\xi^d(K, L)]^{-1}. \tag{6.1}$$

Here C_H is the specific heat at constant magnetic field. In the range $0 < K < K_c$ κ is non-negative definite. Our results for it are shown in figure 6 and are consistent with the idea that

$$\lim_{K\to K_c} \lim_{L\to\infty} \kappa(K, L) > 0. \tag{6.2}$$

All our points should have a systematic error of the order of 1% or smaller, and the statistical errors are again masked by the size of the 'dots'. We conclude that our numerical results are consistent with this hyperscaling relation.

7. Estimates of various critical indices

The main purpose of this article is not to estimate critical indices, however, when we make log–log plots of our data versus $K_c - K$, they tend to be quite straight, with the plot for χ

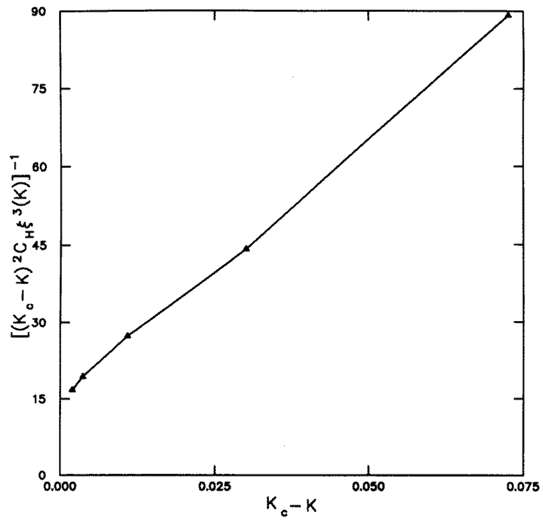


Figure 6. The estimator function for the Josephson relation versus $K_c - K$.

Table 4. Various critical indices

Index	Our results	Reference [20]
γ	1.238(2)	1.241(4)
$\gamma + 2\Delta$	4.41(4)	4.373(14)
ν	0.62(3)	0.630(2)
α	0.18(2)	0.111(6)

the straightest and that for C_H the least straight. The following three-point equation for ψ,

$$1 = z\left(\frac{K_c - K_3}{K_c - K_2}\right)^{-\psi} + (1-z)\left(\frac{K_c - K_1}{K_c - K_2}\right)^{-\psi} \qquad \text{where } z = \frac{\phi(K_2) - \phi(K_1)}{\phi(K_3) - \phi(K_1)} \tag{7.1}$$

is appropriate to a function of the form

$$\phi(K) = A(K_c - K)^{-\psi} + B \tag{7.2}$$

and is a simplified variant of the exponential fitting problem which is straightforward to solve numerically. Our results are displayed and compared with those of the field theory implementation of the renormalization group [20] in table 4. It will be seen that they are all consistent within errors except for the specific heat exponent, α. The errors quoted for our results are the statistical errors associated with the Monte Carlo estimation and do not include possible systematic errors due to taking $\xi_L/L \approx 0.1$ instead of zero, nor do they include errors in the fitting form (otherwise known as corrections to scaling). Our results for γ appear to be quite comparable in accuracy to previous estimates and the log–log plot is quite straight in this case. In the case of α the strong variation, illustrated in figure 6, in our view makes this simple-fitting scheme inappropriate. It appears that A in equation (7.2) should not be treated as a constant here but is strongly varying.

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