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Finite-size scaling study of the equilibrium cluster distribution of the two-dimensional Ising model

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Abstract. We use a very fast and efficient algorithm to study by Monte Carlo methods the equilibrium cluster distribution $C_l(L)$, the mean number of clusters per lattice site containing l particles in a square lattice of L^2 sites, of the two-dimensional Ising model at the critical point. Finite-size scaling theory is then used to analyse the scaling ansatz $C_l(L) = l^{-\tau} f(l^s/L)$, τ and s being critical exponents. The second moment of the cluster distribution $p_2(L) = \Sigma\, l^2 C_l$ is shown to behave as $p_2(L) \sim L^\theta$ with $\theta = 1.895 \pm 0.010$. The effect of corrections to scaling is also discussed.

1. Introduction

Cluster or droplet theories of phase transitions have proved to be a very useful tool when studying critical phenomena near a second-order phase transition (Fisher 1967, Domb 1976, Binder 1976a, Bruce and Wallace 1983) and in nucleation theory (Binder and Stauffer (1976), Penrose and Lebowitz (1979); for a review see Gunton *et al* (1983)). Clusters can be unambiguously defined in lattice systems with short range interactions between particles and have a practical relevance in real systems where they can be related to the grains observed by transmission electron microscopy, for example.

An essential ingredient in all the cluster models is the cluster distribution function $C_l(t)$, the number of clusters per volume unit (or lattice site in a lattice model) containing exactly l particles at time t and its equilibrium value $C_l = \lim_{t\to\infty} C_l(t)$. Different theories lead to different expressions for $C_l(t)$ and C_l, and recent Monte Carlo work has been carried out to distinguish between the different theoretical approaches, both for the dynamical properties (Penrose *et al* 1978, 1984, Marro and Toral 1986, Toral and Marro 1987) and the equilibrium properties (Jan *et al* 1982, Marro and Toral 1983, Cambier and Nauenberg 1986). Series expansions have also been used for the same purpose (Sykes and Gaunt 1976, Gaunt and Brak 1985). One of the key points is the scaling behaviour of C_l near T_c, the critical temperature. Very general phenomenological (Fisher 1967, Binder 1976a) and renormalisation group arguments (Bruce and Wallace 1983) suggest that, in the critical regime, C_l must obey a scaling form. The main discrepancy between the different theories is the exact form for the scaling function and the values of the critical exponents.

After the pioneering work of Fisher, the scaling theory of Binder has been the main step forward in the development of phenomenological models. Bruce and Wallace (1983 and references therein) (see also Sim and Bruce 1985) have developed a more fundamental microscopic theory of clusters in the critical region which contains new

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and very fruitful physical ideas. Their theory is based on the statistical mechanics of droplet configurations controlled by surface tension and it is applicable to members of the Ising universality class in low space dimensions, meaning dimensions d for which $\varepsilon \equiv d-1$ can be considered as a small parameter. The ε expansion on which the theory rests is a serious computational drawback and the question which naturally arises is whether the results of the theory can be trusted for 'physical' dimensions, i.e. $d=2$ or 3. Previous work (Marro and Toral 1983) suggested that Binder's theory can provide a correct description of clusters in the three-dimensional Ising model outside the percolation region. Recent work by Cambier and Nauenberg (1986) also seemed to confirm these results in three dimensions but with different values for the critical exponents; their results for $d=2$ were interpreted as showing a complete failure of the microscopic (Bruce and Wallace) model, but this was in contradiction with other computer simulations (Jan *et al* 1982) and results obtained from the series expansions (Gaunt and Brak 1985).

With all these discrepancies in the results of different studies it seems of some importance to provide further evidence for the success or failure of the different theories. The object of this paper is to analyse by Monte Carlo methods the scaling properties of the equilibrium cluster distribution for the two-dimensional Ising model using finite-size scaling theory. To this end, simulations at the critical point for a square Ising lattice were carried out using a very fast algorithm which allows us to overcome the problems originating in the very large correlation times and the critical slowing down at the critical point. Our results are restricted to zero magnetic field.

The outline of the paper is as follows. In § 2 we review briefly the main theoretical results needed to understand the rest of the paper. Section 3 is devoted to a detailed description of the algorithms used in the simulation. Section 4 presents the simulation data and the results concerning the values of the critical exponents and their comparison with theory. None of the existing theories seems to account for the values we obtain in this paper and *ad hoc* modification of the phenomenological theory is presented in order to accommodate them. Finally, § 5 summarises the results.

2. Theoretical models

We refer for simplicity to the ferromagnetic Ising model with nearest-neighbour interactions. A spin variable $S_i = \pm 1$ is located at each of the $N\,(=L^d)$ sites of a d-dimensional regular lattice. The energy of a given configuration is defined by

$$E = -J \sum_{\mathrm{NN}} S_i S_j \qquad J>0 \tag{2.1}$$

where the sum runs over all the nearest-neighbour pairs of sites. In this model, a cluster can be unambiguously defined as a maximal connected set of, say, down spins ($S_i=-1$), i.e. a cluster is a set of sites occupied by down spins in the latttice which are mutually connected by at least one nearest-neighbour bond (we will not discuss here the problems associated with the presence of percolation which appears for densities smaller than the critical one in three or more dimensions; relevant clusters should then be defined in some other way; see Binder (1976a), Coniglio and Klein (1980), Heermann *et al* (1984)). The size l of a cluster is then simply defined as the number of sites which belong to it. The equilibrium number of l-particle clusters per site of the lattice is denoted by C_l. The system magnetisation $m \equiv N^{-1}\Sigma_i S_i$ is then

given by the exact relation (sum rule)

$$m = 1 - 2 \sum_{l=1}^{\infty} l C_l. \tag{2.2}$$

The scaling form satisfied by the magnetisation m near T_c, the critical temperature, and the above sum rule are the basis for a scaling description of the equilibrium cluster distribution function C_l itself. Such scaling behaviour was introduced by Fisher (1967) in a more general study on the nature of the singularities of the thermodynamic potential at the condensation point and it was substantially extended by Binder (1976a). The Fisher-Binder (FB) scaling result for C_l near T_c (and zero magnetic field) states that near (and below) the critical temperature

$$C_l = l^{-\tau} f_1(tl^s) \tag{2.3}$$

$t \equiv 1 - T/T_c$ is the reduced temperature (no confusion should arise in practice with 't' meaning 'time'), $f_1(x)$ is the scaling function and the critical exponents τ and s are given in terms of the standard exponents β and δ which characterise the behaviour of the magnetisation in the critical region by

$$\tau = 2 + y/\delta \tag{2.4a}$$

$$s = y/\beta\delta. \tag{2.4b}$$

y is a free parameter in this theory such that l^y is a measure of the effective magnetisation of an l cluster (Binder 1976a) (the original Fisher model assumes $y = 1$ and gives an explicit expression for the function $f_1(x)$).

To derive (2.4) from (2.3) one needs to match the exponents of the power law behaviour of both sides of (2.2). The left-hand side behaves near T_c as

$$m = m_0 t^{\beta}. \tag{2.5}$$

The matching is more easily done by differentiating equation (2.2) (so that the dominant terms in both sides of the equation diverge as $t \to 0$):

$$\frac{\partial m}{\partial t} = -2 \sum_{l=1}^{\infty} \frac{\partial C_l}{\partial t}. \tag{2.6}$$

Inserting expressions (2.3) and (2.5) and converting the sum into an integral (which is justified in the critical regime where $t \to 0$) we have

$$m_0 \beta t^{\beta - 1} = -2 \int_1^{\infty} \mathrm{d}l \, l l^{-\tau} l^s \frac{\mathrm{d}f_1(x)}{\mathrm{d}x} \tag{2.7}$$

where $x = tl^s$. This can be written as

$$m_0 \beta t^{\beta - 1} = -2 s^{-1} t^{(\tau - 2)/s - 1} \int_t^{\infty} \mathrm{d}x \, x^{(2-\tau)/s} \frac{\mathrm{d}f_1(x)}{\mathrm{d}x} \tag{2.8}$$

leading to the identification $\beta = (\tau - 2)/s$, which is equivalent to (2.4).

A more microscopic theory has been developed by Bruce and Wallace (1983, hereafter referred to as BW). Their theory studies the configurational physics underlying the critical phenomena for systems belonging to the Ising universality class. The main result for the equilibrium cluster distribution is that it obeys a scaling form

$$C_l = l^{-\tau} f_2(l^{s\nu}/\xi) \tag{2.9}$$

where ξ is the correlation length (this equation comes out when one rewrites equation (5.20) of BW in terms of the dressed volume of a cluster). τ and s are critical exponents completely determined (see later) and $f_2(x)$ is a scaling function explicitly given by BW in a perturbative approach. Given that $\xi \sim t^{-\nu}$ in the critical region, the scaling ansatz (2.3) is recovered and the exponents are explicitly given by

$$\tau = 2 + \psi_0/(d - \psi_0) \tag{2.10}$$

$$s = [(d - \psi_0)\nu]^{-1} \tag{2.11}$$

where $\psi_0 = \beta/2\nu$ so that $(\tau - 2)/s = \beta/2$, at variance with (2.4). A contradiction arises when one thinks that (2.4) seems to be mandatory given the scaling form (2.3) and the (exact) sum rule (2.2). What BW showed is that, at least within their explicit theory, the integral appearing on the right-hand side of (2.8) vanishes in the critical region (specifically it behaves as $t^{\beta/2}$) so that (2.4) is not a necessary conclusion of (2.3) and (2.2). There is no *a priori* simple physical justification of this second sum rule that dictates that the integral in (2.8) vanishes, but this marks the difference (from a practical point of view) between the BW and FB theories of droplets.

Very large statistical fluctuations in the number of large clusters present in the system make it very difficult to measure accurately the cluster distribution C_l in a MC simulation. Better statistics can be derived from the study of the moments of the cluster distribution. In particular, the second moment is defined by

$$p_2(t) = \sum_{l=1}^{\infty} l^2 C_l \tag{2.12}$$

(this is the lowest-order moment with a divergent behaviour in the critical regime). Substituting (2.3) and converting the sum into an integral, we obtain that $p_2(t)$ diverges as

$$p_2(t) \sim t^{-\theta} \tag{2.13}$$

with

$$\theta = (3 - \tau)/s = \beta(\delta/y - 1) \tag{2.14}$$

in the FB theory, or

$$\theta = (3 - \tau)\nu/s = d\nu - \beta = \gamma + \beta \tag{2.15}$$

in the BW theory (we have used the hyperscaling relation $2\beta + \gamma = d\nu$). In two dimensions (2.15) leads to $\theta = 1.875$ whereas the original Fisher model ($y = 1$) predicts $\theta = \beta(\delta - 1) = \gamma = 1.75$ and p_2 is associated with the magnetic susceptibility. We want to stress that (2.13) refers to the behaviour of an infinite system when approaching criticality. In § 4, on the other hand, finite-size scaling theory will be used to study the corresponding behaviour of finite systems.

3. Simulation details

The ICL distributed array processor (DAP) is the machine which has been used to perform the numerical investigations described. The DAP is an example of a single instruction multiple data (SIMD) parallel processing computer. This means that the machine can simultaneously perform the same operation on many different pieces of

data held in its store. The DAP hardware consists of what can be thought of as a square array of 64×64 processing elements (PE), each of which is connected to its four nearest neighbours. Data can hence be passed from processor to processor via these nearest-neighbour connections, which is very important for shift operations. Each processor is very basic and operates on data bit by bit. The 4096 processors constitute the PE matrix. Associated with each processor are 4096 bit of memory so that the plane of processors has 4096 bit planes of memory above it collectively forming the DAP store, in which the coded instructions and data on which they are to act (constituting the software) are stored.

The 4096 processing elements arranged as a 64×64 matrix enable the DAP to process data in parallel in its store. Each PE can perform simple logical operations on operands that are single bit values. These characteristics make the DAP very efficient for Ising model simulations, since one can map every lattice site into a PE which is then connected in a natural way to the four neighbours as the sites in a square lattice are. By using the DAP assembly language (APAL), Reddaway *et al* (1985) have written the fastest program to date to simulate the Metropolis algorithm for the simulation of the canonical ensemble of the three-dimensional Ising model (with 218 million spin updates per second). We are indebted to D M Scott for providing us with a copy of this program which has been conveniently modified and optimised by us to deal with the two-dimensional Ising model. The main feature of the algorithm is parallel updating. That is, all the sites which are not connected by a nearest-neighbour relationship (half of the lattice for a square lattice) are updated simultaneously using the Metropolis method. This procedure satisfies all the requirements of ergodicity and approach to the equilibrium of the standard Metropolis algorithm (see, for instance, Binder 1976b) but obviously it is much faster than a serial update. The DAP hardware and software then provide a natural scenario for the simulation of the parallel update realisation of the Metropolis algorithm for the 64^2 Ising model. The boundary conditions (either periodic or free) are provided 'free' in the hardware. Using more complicated mappings, smaller and larger systems can be simulated as well. It turns out that, in order to maximise the program efficiency, the side of the system has to be a power of two. We therefore studied in this work system sides with $L = 4$, 8, 16, 32, 64 and 128. It is then possible to have independent simulations running at the same time; for a given side L, the number of independent simultaneous simulations is $(128/L)^2$ and is given in table 1.

Table 1. Simulation details.

Side	4	8	16	32	64	128
Number of runs	1 024	256	64	16	4	1
Number of measurements in every run	40 000	50 200	56 100	53 100	57 330	28 254
MC steps between measurements	100	250	1 000	5 000	25 000	100 000
MC steps discarded for equilibration	2 000	5 000	10 000	50 000	250 000	1000 000

Obtaining the cluster size distribution implies labelling all the sites belonging to the same cluster and updating the labels each time two candidate clusters happen to be connected. In such a process the parallelism of the DAP cannot be used efficiently. A different approach has been taken. We have used an 'ant algorithm' in which an occupied site of the lattice is selected, and then by means of logical operations and shifts it is propagated in all directions labelling the occupied neighbour sites which belong to the same cluster as the original site; the labelled sites then propagate in the

same way as the initial site. When no further expansion is possible, the cluster size is recorded and the cluster is removed from the system. The algorithm is then repeated until no more clusters are present. This routine analyses the clusters one by one and the parallelism of the DAP is still not fully exploited. Even though a complete parallel algorithm that keeps track of all the clusters simultaneously is possible (Toral 1986) it involves integer arithmetic and is not as fast as the 'ant algorithm' described before. The routine is capable of analysing more than 250 000 random configurations per hour in a 32×32 lattice. Since the clusters are analysed individually, the fewer the clusters, the more efficient the ant algorithm is. The actual number of configurations analysed per hour at the critical temperature (where a spanning cluster is present most of the time) is then larger than the number of random configurations analysed in the same time.

The requirement of this numerical investigation is to obtain unbiased estimates for canonical ensemble averages of different magnitudes, say $\langle A \rangle_{K,L}$, for the pure spin-$\frac{1}{2}$ Ising model on a square lattice with periodic boundary conditions and linear extent L. To sufficient accuracy such estimates should allow finite-size scaling theory to be scrutinised at K_c ($= 0.440\,686\ldots$ for the square 2D Ising model), where the finite-size precursors of the critical phenomena associated with the infinite system are expected to appear. The rest of this section is devoted to describing how our Monte Carlo simulation overcomes the difficulties associated with this requirement. A description of the parallel implementation of the Metropolis algorithm and its dynamical properties can be found in the papers by Williams (1985a, b).

In MC importance sampling, a Markov process or algorithm is sought and used to update configurations in such a way that configuration $\{S\}$ appears with the desired frequency $\exp(-\beta H(\{S\}))/Z$. In this way the Boltzmann probability weighted average is replaced by a numerical average of $A(\{S\})$ measured on MC generated configurations appearing with frequencies proportional to their 'importance'. Whatever the specific implementation of the algorithm, the number of MC steps (where one MC step is one sweep of the whole lattice) required for this Markov process to reach a regime where configurations are appearing with frequency $\exp(-\beta H(\{S\}))/Z$ (i.e. the equilibration time) and the time taken for such configurations to be forgotten, or completely changed (i.e. the relaxation time), are particularly important properties of the updating algorithm. The lower limit on these times is set by the Hamiltonian simulated. The critical slowing down, critical increase of relaxation times and increased fluctuations associated with the fluctuations of cooperating degrees of freedom on all length scales near criticality arise for the dynamic Ising model and, via the interpretation of the MC dynamics as Ising model dynamics, also arise for the Metropolis algorithm (see, e.g., Binder 1976b, Tobochnik *et al* 1981, Williams 1985b). Here the results are used to obtain *a priori* estimates for the run times necessary to measure the quantities of interest to a given statistical accuracy. In particular, we are interested in finding how many MC steps, N_{in}, we need to discard at the beginning in order to reach equilibrium, and how many MC steps, N_{upd}, are necessary to update the system from a configuration to an independent one. In order to perform tests on large system sizes, N_{upd}, N_{in} and N_{mes} (the number of independent measurements) must be optimised to offset the problems of critical slowing down, long time transients, increased fluctuations and increased system size. Due to all these problems, MC simulations typically avoid the critical region where large relaxation times imply large CPU times (and a big monetary cost). This is the main reason for the need of a fast algorithm.

Let us discuss first the value of N_{upd} as a function of the side L. For a finite system, the relaxation time increases as L increases but, of course, remains finite (although

very large) at $T = T_c$. More specifically, if the relaxation time for the decay of an observable A is denoted by τ_A, critical slowing down states that near T_c

$$\tau_A = \tau_A^0 |1 - T/T_c|^{-\Delta_A}. \tag{3.1}$$

Finite-size scaling theory implies then that the relaxation time for a finite system of linear extent L at $T = T_c$ scales as

$$\tau_A(L) = \hat{\tau}_A^0 L^{z_A} \tag{3.2}$$

where $z_A = \Delta_A/\nu$. In the Metropolis dynamics the largest relaxation time is associated with the magnetisation m. The criterion to estimate the number of MC steps necessary to get an independent configuration is then given by the condition

$$N_{\text{upd}}(L) \gg \tau_m(L) \tag{3.3}$$

(τ_m is measured in MC units, 1 MC unit being equal to one lattice sweep). The parallel update has its own relaxation time (which is, in principle, different from the relaxation time of the serial update). An estimate for $\tau_m(L)$ has been given by Williams (1985a). He computed the magnetisation autocorrelation function for the Metropolis algorithm of the 2D Ising model at T_c:

$$\Gamma(L, t) = N^{-1} \left\langle \sum_i S_i(0) S_i(t) \right\rangle. \tag{3.4}$$

For large time t, $\Gamma(L, t)$ presents an exponential decay $\Gamma(L, t) = a(L) \exp(-\lambda(L)t)$. $\lambda^{-1}(L)$ is identified with τ_m (for a detailed justification of this fact see Williams (1985a)) and then fitted to the power law

$$\lambda^{-1}(L) = CL^z \tag{3.5}$$

with $C = 0.91$ and $z = 2.1$. In our simulation, the condition (3.3) has been fulfilled by taking N_{upd} to be roughly four times $\lambda^{-1}(L)$. The actual values of N_{upd} for the different system sizes are given in table 1. The excellent agreement between the exact known values of some magnitudes and the ones measured in the simulation are an *a posteriori* test that the configurations are indeed statistically independent.

The number of configurations discarded for equilibration is dictated by the condition

$$N_{\text{in}} \gg \tau_m^{\delta K} \tag{3.6}$$

where $\tau_m^{\delta K}$ is the characteristic equilibration time for the magnetisation m for an initial configuration whose equilibrium inverse temperature deviates by an amount δK from the desired equilibrium. The critical slowing down of the equilibration time is described by

$$\tau_m^{\delta K} = \tau_{m,0}^{\delta K} |1 - T/T_c|^{-\Delta_m^{\delta K}} \tag{3.7}$$

where $\Delta_m^{\delta K}$ is a dynamic critical exponent. This implies, via finite-size scaling, that at T_c:

$$\tau_m^{\delta K} \sim L^{\Delta_m^{\delta K}/\nu} \tag{3.8}$$

so that for a finite system the necessary equilibration increases dramatically with system size. In all our runs we have used hot starts corresponding to an initial value $K_0 = 0$ and so $\delta(K) = K$. τ_m^K can be approximated by the time the system takes to reach one of the ground states from the initial (random) configuration. It turns out that $\tau_m^K \ll \tau_m$ for all the sizes studied here. However, to make sure that the equilibrium regime has been reached, N_{in} was chosen as $10 N_{\text{upd}}$ (in that time the system has typically oscillated about 30 times from one ground state to the other). The actual values are in table 1.

4. Simulation results

Several magnitudes were recorded in the simulation. The energy values, u, defined as the number of up-down bonds per lattice site and its fluctuations, $\sigma_u^2 \equiv \langle u^2 \rangle - \langle u \rangle^2$ (proportional to the specific heat), agree perfectly (see table 2) with the known exact results for the finite 2D Ising model (Kaufman 1949, Ferdinand and Fisher 1969). This agreement between the simulation and the exact results is strong evidence that the number of MC steps between two different measurements was large enough to generate independent configurations. We believe it is appropriate to present these results in detail because this is the first time that the algorithm (which involves a new method of generating random numbers, see Smith *et al* (1985)) has been tested against exact known results. We also computed the magnetisation m and its fluctuations, $\chi^*(L) \equiv L^2\sigma_m^2$, with $\sigma_m^2 \equiv \langle m^2 \rangle - \langle m \rangle^2$ (χ^* is proportional to the magnetic susceptibility). The simulation data are given in table 2. The exact expression for χ^* is not known for a finite lattice of general size (exact results were generated by direct enumeration for systems with lattice side up to 4), but the simulation values can be used to compute the known ratio of critical exponents γ/ν. If finite-size scaling holds for the sizes we are dealing with, we should get $\chi^*(L) = \chi_0 L^{\gamma/\nu}$ with $\gamma/\nu = 1.75$. In the logarithmic plot of figure 1, we see that this simple power law behaviour is valid (surprisingly) even for small values of L. A least squares fit to the 'susceptibility' χ^* data for $4 \leq L \leq 128$ yields $\gamma/\nu = 1.76 \pm 0.02$. This is an additional test that our simulation gives the correct values for the critical exponents.

Table 2. Comparison of the results of the simulation with exact results for the two-dimensional Ising model. The numbers in brackets are the (statistical with one standard deviation) errors which affect the last digits of every measurement. The mean value of the magnetisation was zero within the statistical errors for all the lattice sizes.

Side	4	8	16	32	64	128
u (exact)	0.217 188 ...	0.254 205 ...	0.273 468 ...	0.283 171 ...	0.288 031 ...	0.290 46 ...
u (simulation)	0.217 205 (38)	0.254 227 (42)	0.273 418 (46)	0.283 136 (52)	0.287 960 (55)	0.290 17 (10)
C_v (exact)	0.52	1.474 68 ...	1.929 ...	2.377 ...	2.822 ...	3.265 ...
C_v (simulation)	0.520 28 (43)	1.468 3 (93)	1.942 (12)	2.366 (15)	2.820 (17)	3.252 (27)
$L^2\sigma_M^2$ (exact)	12.181 7 ...					
$L^2\sigma_M^2$ (simulation)	12.184 4 (41)	41.48 (26)	140.03 (84)	477.4 (2.9)	1593.0 (9.4)	5380 (45)

We turn now to the cluster distribution function. Let us study first the second moment $p_2(L)$, defined in (2.12), as a function of the side L. The exact values of $p_2(L)$ have been obtained by direct enumeration of all the possible states for side less than or equal to 4. Table 3 lists the exact and the simulation results. Excluding the largest value of $L = 128$, the errors are less than 0.2%. A least squares fit to the single scaling law $p_2(L) = CL^\theta$ (see figure 2) for $4 \leq L \leq 128$ gives the values $C = 0.5068$, $\theta = 1.896$ (even $p_2(L = 1)$ is well approximated by the fit!), with a correlation coefficient $r = 0.999\,9993$. Obviously, this is an excellent fit but it does not take into account the possibility of the presence of correction to scaling terms, which are present indeed in the scaling description of $p_2(L)$. How important (from a numerical point of view) are the correction to scaling terms? Three different methods have been used to study the possible influence of these terms.

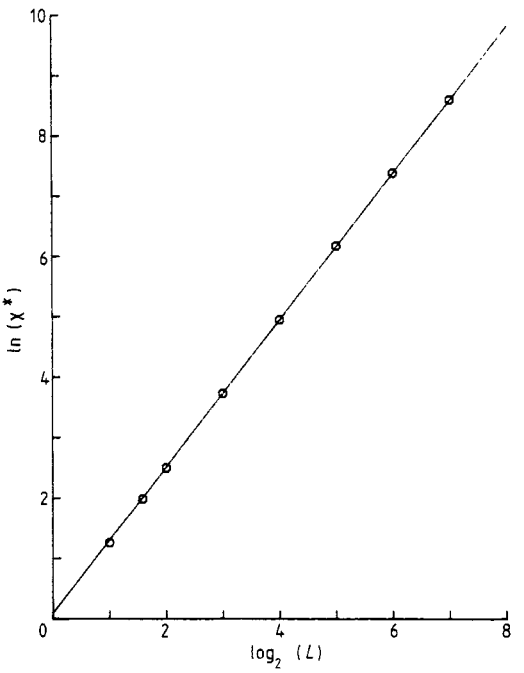

Figure 1. Logarithmic plot of $\chi^* = L^2\sigma_m^2$ (χ^* is proportional to the magnetic susceptibility) against L, system side (the x axis is the base 2 logarithm of L, and the y axis the natural logarithm of χ^*). The (statistical) errors are smaller than the size of the symbols. The straight line is the asymptotic behaviour $\chi^* \sim L^{\gamma/\nu}$, $\gamma/\nu = 1.75$ (exact value for the two-dimensional Ising model). A least squares fit to the data gives $\gamma/\nu = 1.76 \pm 0.02$ in perfect agreement with the exact result. Even though the fit is very good, a closer analysis shows that some kind of correction to scaling terms are necessary for small values of L, say $L < 2^4 = 16$.

Table 3. Values of $p_2(L)$, second moment of the equilibrium cluster distribution, as a function of L, the lattice side. The values are exact for $L < 4$.

L	$p_2(L)$
1	0.5
2	1.873 896 10...
3	4.068 869 87...
4	7.034 502 27...
8	26.145 4 (73)
16	97.131 (51)
32	360.62 (39)
64	1343.5 (2.8)
128	5035 (45)

Firstly, we have looked for any trend in the set of critical exponents deduced from any pair of values of $p_2(L)$. To this end, let us define

$$\theta(L_1, L_2) = \frac{\ln\{p_2(L_2)/p_2(L_1)\}}{\ln(L_2/L_1)}. \tag{4.1}$$

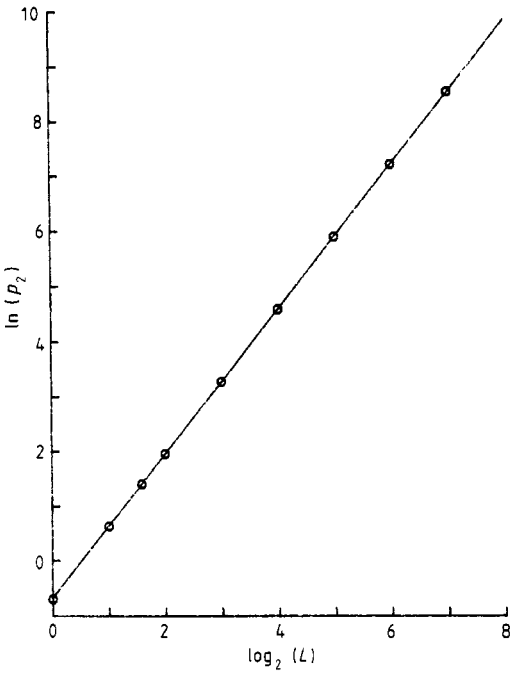

Figure 2. Plot of the natural logarithm of the second moment of the cluster distribution $p_2(L) = \Sigma_l l^2 C_l(L)$ against the logarithm in base 2 of the lattice side L. The errors are smaller than the symbol size. The line shows the behaviour $p_2(L) \sim L^\theta$ with $\theta = 1.895$ obtained by a least squares fit to the data and other methods (see text). Again, as in figure 1, some kind of correction to scaling terms are required for small L, say $L < 2^3 = 8$.

Table 4 shows the values of $\theta(L_1, L_2)$ for all the possible sets of couples (L_1, L_2) (the same table includes the results of a similar analysis for the magnetic susceptibility). It is clear from this table that small values of L_1 and/or L_2 produce values of $\theta(L_1, L_2)$ different from those generated by large L values (which are presumably closer to the true asymptotic value). On the other hand, no systematic trend is observed when $L_2 > L_1 > 4$. This suggests that we have reached the asymptotic regime where correction

Table 4. The upper-right half is a table of $\theta(L_1, L_2)$ as defined in equation (4.1) for all the possible pairs of L_1 and L_2. When $L_2 > L_1 > 4$, the $\theta(L_1, L_2)$ stabilise around the value $\theta = 1.896$. The lower-left half is a similar table for the critical exponent γ of the magnetic susceptibility. The exact result in this case is $\gamma = 1.75$.

	L_1							
L_2	2	3	4	8	16	32	64	128
1	1.906 04	1.908 33	1.907 22	1.902 83 (13)	1.900 46 (19)	1.888 87 (31)	1.898 63 (50)	1.9000 (18)
2		1.912 24	1.908 41	1.901 22 (20)	1.898 61 (25)	1.897 07 (39)	1.897 15 (60)	1.8986 (21)
3	1.809 96		1.903 01	1.896 67 (28)	1.895 30 (31)	1.894 48 (46)	1.895 15 (68)	1.8972 (24)
4	1.800 51	1.787 18		1.894 04 (40)	1.893 71 (38)	1.893 30 (52)	1.894 33 (75)	1.8967 (26)
8	1.784 1 (45)	1.773 4 (64)	1.767 7 (90)		1.893 4 (12)	1.892 93 (98)	1.894 4 (11)	1.8973 (33)
16	1.774 5 (29)	1.765 9 (36)	1.761 5 (43)	1.755 (18)		1.892 5 (23)	1.895 0 (19)	1.8986 (46)
32	1.773 2 (22)	1.766 9 (26)	1.764 1 (29)	1.762 4 (89)	1.770 (18)		1.897 4 (46)	1.9017 (72)
64	1.766 3 (17)	1.760 5 (19)	1.757 7 (21)	1.754 4 (59)	1.754 0 (86)	1.739 (18)		1.906 (16)
128	1.764 5 (20)	1.759 6 (22)	1.757 3 (24)	1.754 8 (53)	1.754 6 (69)	1.747 (11)	1.756 (21)	

to scaling terms are of little numerical importance. The average of the $\theta(L_1, L_2)$ values for this table when $L_2 > L_1 > 4$ is 1.896(4), the error defined as one standard deviation. Other procedures to find trends in the data, like a least squares fit from an initial L_{in} to $L = 128$ with different values of L_{in} or fitting in triplets of L values, also lead to similar conclusions. Figures 3 and 4 plot the diagonal values of table 4 for the effective critical exponents for χ^* and p_2 respectively against $1/L$. Extrapolating towards the origin gives estimates of γ/ν and θ/ν as 1.75 ± 0.02 and 1.895 ± 0.010.

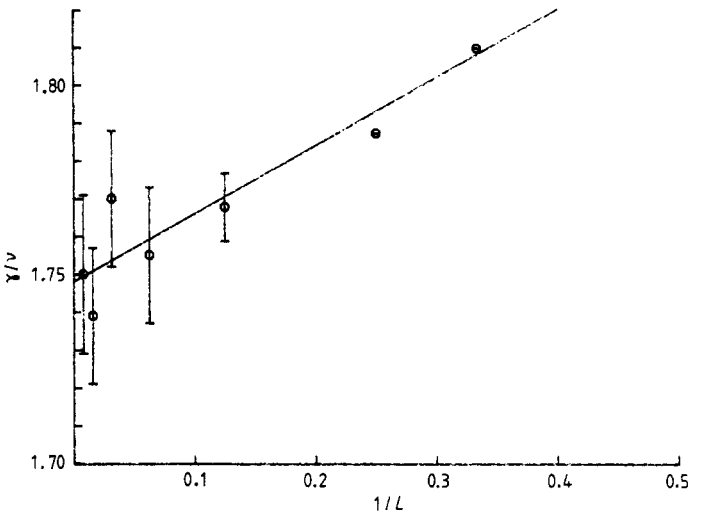

Figure 3. Plot of the 'diagonal' values of table 3 corresponding to the effective exponents obtained by fitting a power law to the susceptibility data for different values of L, the system side. The full line is a straight line fit to the points. The limiting value when $1/L = 0$ is consistent with the exact value $\gamma/\nu = 1.75$.

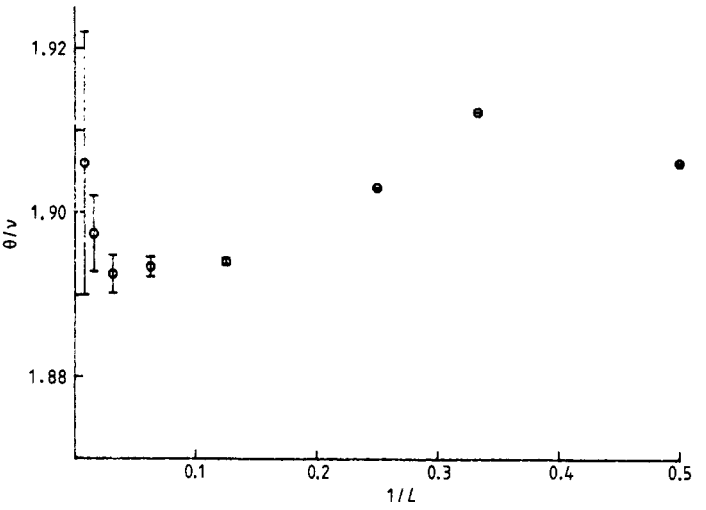

Figure 4. Similar to figure 3, but for the effective exponents of the second moment of the cluster distribution. This figure is a strong support for our value $\theta/\nu = 1.895 \pm 0.010$.

Secondly, we have applied extrapolation methods (see Barber 1983 and references therein), to accelerate the convergence of $\theta(L_2, L_1)$ to the asymptotic value θ. We are aware that our data are not precise enough to use acceleration techniques in order to get a very precise estimate of the asymptotic value θ, but we use them in order to have an independent estimate of the errors. The simplest correction to scaling term that can appear in $p_2(L)$ is of the form

$$p_2(L) = CL^{\theta}(1 + BL^{-\omega}) \tag{4.2}$$

or introducing n such that $L = 2^n$

$$p_2(n) = C2^{n\theta}(1 + B2^{-n\omega}). \tag{4.3}$$

Let us define $\theta_n = \theta(2L, L) = \ln[p_2(n+1)/p_2(n)]/\ln(2)$. Equation (4.3) implies the asymptotic behaviour $\theta_n = \theta + ab^{-n}$. If this expression holds then, starting from some initial values $\theta_n^{(0)}$, the combination

$$\theta_n^{(1)} = \frac{\theta_n^{(0)}\theta_{n+2}^{(0)} - (\theta_{n+1}^{(0)})^2}{\theta_{n+2}^{(0)} - 2\theta_{n+1}^{(0)} + \theta_n^{(0)}} \tag{4.4}$$

should be independent of n. Iterating this process, we obtain a series of estimates $\theta_n^{(i)}$ whose dispersion gives some idea about the final errors in the estimate of θ itself. Table 5 shows the results of this acceleration scheme. This leads again to $\theta = 1.895(10)$. More sophisticated acceleration techniques are available (Barber and Hamer 1982) and when used they give the same value for θ.

Table 5. A method of accelerating the convergence of the magnitudes $\theta_n^{(0)} \equiv \ln[p_2(2^{n+1})/p_2(2^n)]/\ln 2$. They are shown to behave as $\theta_n^{(0)} = \theta + ab^{-n}$. Defining $\theta_n^{(i)} = [\theta_n^{(i-1)}\theta_{n+2}^{(i-1)} - (\theta_{n+1}^{(i-1)})^2](\theta_{n+2}^{(i-1)} - 2\theta_{n+1}^{(i-1)} + \theta_n^{(i-1)})^{-1}$ the $\theta_n^{(i)}$ represent a better estimate of the magnitude θ for increasing values of i.

n	$\theta_n^{(0)}$	$\theta_n^{(1)}$	$\theta_n^{(2)}$	$\theta_n^{(3)}$
0	1.906 04	1.906 37	1.895 28	1.8951
1	1.908 41	1.893 37	1.894 47	
2	1.894 04	1.895 62	1.896 75	
3	1.893 4	1.893 26		
4	1.892 5	1.886 01		
5	1.897 4			
6	1.906			

Thirdly, we have tried to fit directly an expression containing the expected form of the correction to scaling terms to $p_2(L)$. Following Gaunt and Brak (1985) we write down an expression that includes the possible appearance of analytic and non-analytic correction to scaling terms (Aharony and Fisher 1980, 1983). In the bulk, they contribute as

$$p_2(L = \infty, T \to T_c) = Ct^{\theta}\{1 + At^{\Delta} + Bt\}. \tag{4.5}$$

The exponent Δ has been calculated to be $\Delta = 1.3$ (Le Guillou and Zinn-Justin 1980) for the 2D Ising universality class. Finite-size scaling theory then predicts that

$$p_2(L, T_c) = CL^{\theta}\{1 + AL^{-\Delta} + BL^{-1}\} \tag{4.6}$$

(the constants A, B, C take different values in expressions (4.5) and (4.6)). Defining $y = p_2L^{-\theta}$, $x = L^{-1}$, we tried to get the parameters of the best fit to $y = C(1 + Bx + Ax^{\Delta})$.

It is very difficult to try to determine Δ from the simulation data (for a given θ there are four parameters in equation (4.6) and we have at most nine pairs of data $(L, p_2(L))$ for L ranging from 1 to 128; to use $L = 1$, 2 and 3 is probably nonsense and that leaves us with only six pairs of data to try to fit four parameters!). Assuming $\Delta = 1.3$ the best fits are reproduced in figure 5 for $\theta = 1.895$ and $\theta = 1.875$, the mean relative error of the fits being 3×10^{-3} and 9×10^{-3} respectively. These errors and figure 5 show that $\theta = 1.895$ produces a much better fit to the data. When $\theta = 1.875$ the values on the vertical axis in figure 5 do not stabilise and corrections to scaling seem to be required for large values of L, which is unlikely. With the above evidence we give our estimate of θ as

$$\theta = 1.895 \pm 0.010. \tag{4.7}$$

The error quoted is subjective (as many errors in Monte Carlo simulations are) but it covers all the values of θ deduced from the different methods explained previously and we really believe that it is a generous estimate for the error. Let us emphasise, however, that the data analysis leading to (4.7) rests upon the scaling form (4.6). If (4.6) is wrong, i.e. if other correction to scaling terms numerically important ought to be present in (4.6) (i.e. logarithmic corrections, see Barma and Fisher (1985)) then the value (4.7) for θ could be modified. However, this seems to us a very unlikely possibility. On the other hand, if only analytic correction to scaling terms are present in (4.6) (i.e. if $\Delta = 2$) the estimate (4.7) remains unchanged.

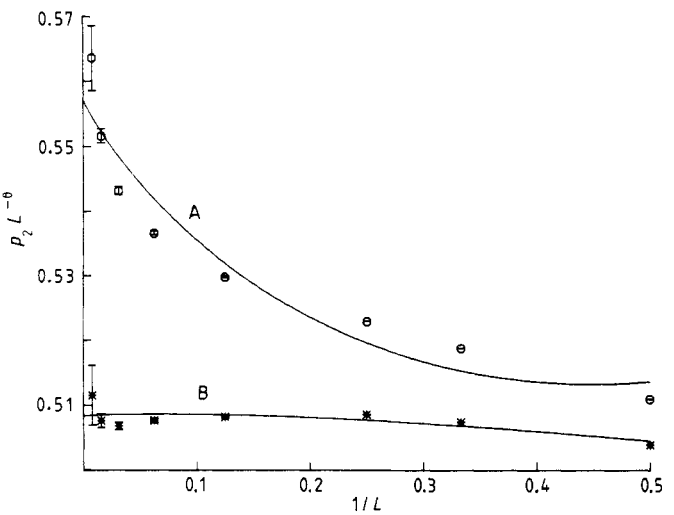

Figure 5. Plot of $p_2(L)L^{-\theta}$ against $1/L$ for two different values of θ: 1.875 (A) and 1.895 (B). The full curves represent the best fit of equation (4.6) to the simulation data.

Let us now analyse directly the scaling ansatz (2.3). As already commented, the statistical errors in C_l do not allow us to obtain conclusions concerning the critical exponents as precise as the ones we obtained with the second moment $p_2(L)$. But other very interesting results follow. As formulated, (2.3) applies to infinite systems near the critical temperature. Standard finite-size scaling theory (Barber 1983) tells us what form for the scaling law we should expect for a finite system at the critical

temperature of the infinite system:

$$C_l(L) = l^{-\tau} f_4(l^s/L^\nu) \tag{4.8}$$

(in the 2D Ising model $\nu = 1$). This is equivalent to writing

$$\ln C_l(L) + (\tau/s)\ln L = f(\ln l - (1/s)\ln L) \tag{4.9}$$

where $f(x)$ is a scaling function independent of L in the scaling regime (for large enough values of L). The BW values for the critical exponents are (see § 2) $\tau = 2+\beta/(2d\nu-\beta) = \frac{63}{31}$ and $s = (d\nu - \nu/2)^{-1} = \frac{16}{31}$ in two dimensions. We see in figure 6 that the scaling function $f(x)$ derived using these values for the critical exponents is indeed L independent, at least within the accuracy of the simulation data. In the FB theory, the undetermined parameter y can be related to the exponent θ of the divergence of the second moment of the cluster distribution by $y = \delta/(1+\theta/\beta)$ (see § 2). The value (4.7) for θ yields $y = 0.9282(46)$ and then, according to equations (2.4), $\tau = 2.061\,88(31)$ and $s = 0.4950(25)$. In figure 7 we plot the function $f(x)$ derived from these values of τ and s. It is clear that the scaling, although it is reasonably good, is not as good as the one obtained in figure 6. The data seem to prefer the BW description to the FB one in two dimensions. We thus have the situation where neither of these two theories can explain fully the values of the critical exponents *and* the scaling function derived in this paper.

We now present an *ad hoc* modification of the phenomenological theory in order to cope with the simulation results. The modification consists of incorporating the sum rule that holds within the BW theory that states that the integral on the right-hand side of equation (2.8) vanishes near the critical point as $t^{\beta/2}$. The relation between the critical exponents is then modified to

$$\beta/2 = (\tau - 2)/s \tag{4.10}$$

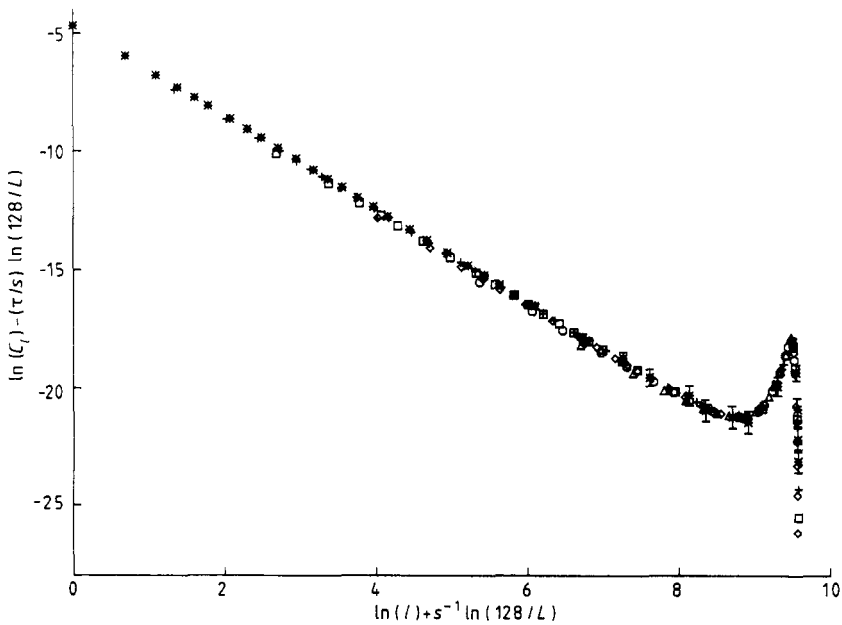

Figure 6. Scaling test of the ansatz $C_l = l^{-\tau} f(l^s/L)$ with the values of $\tau(\frac{63}{31})$ and $s(\frac{16}{31})$ predicted by the BW theory (see text) $l = 4$ (△); 8 (◯); 16 (◇); 32 (□); 64 (+); 128 (*).

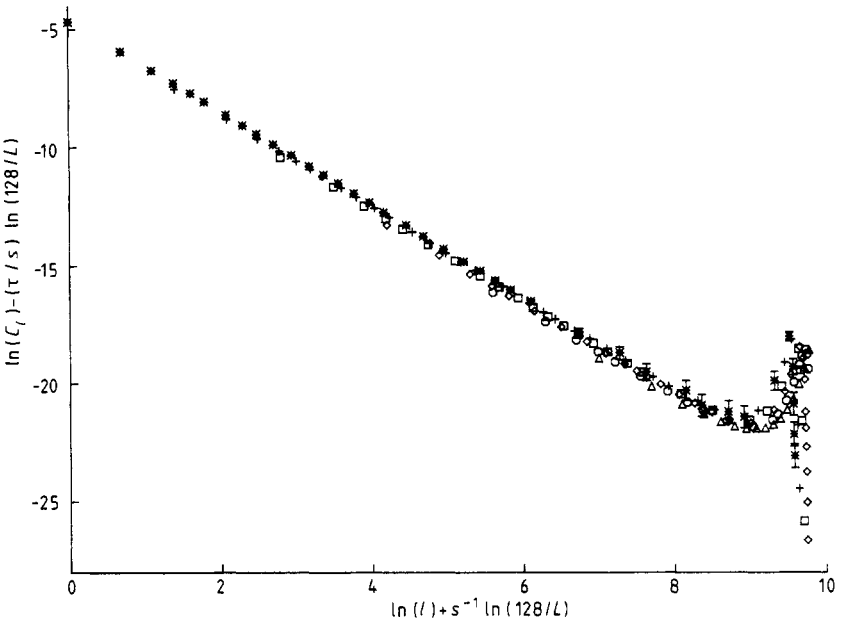

Figure 7. Same as figure 6, but the values of the critical exponents τ and s are those deduced from the Binder theory, namely $\tau = 2 + y/\delta$, $s = y/\beta\delta$, with $y = 0.9282$ (see the text for an explanation of this y value).

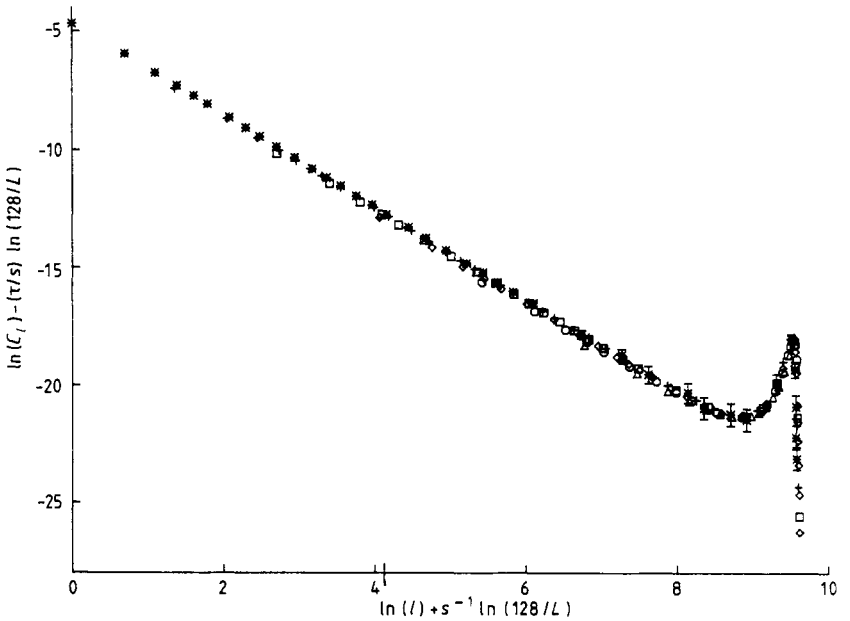

Figure 8. Same as figure 6, but τ and s are given by $\tau = 2 + y/2\delta$, $s = y/\beta\delta$, with $y = 0.9579$ (see text).

and introducing a new parameter y', (4.10) is equivalent to the pair of equations

$$\tau = 2 + y'/2\delta \tag{4.11a}$$

$$s = y'/\beta\delta. \tag{4.11b}$$

(The numerical results of the BW theory are contained in equations (4.11) since the BW values for the exponents τ and s can be written in the form (4.11) with $y' = \frac{30}{31}$.) The exponent of the critical divergence of p_2 is then given by $\theta = \beta(\delta/y' - \frac{1}{2})$ and from (4.7) we deduce $y' = 0.9579(49)$ and (4.11) yields $\tau = 2.031\,93(16)$, $s = 0.5109(26)$. Figure 8 shows that the scaling function $f(x)$ deduced with these values of τ and s is L independent. We conclude then that the scaling form (2.3) together with the exponents τ and s given by (4.11) are an excellent description of the critical behaviour of the cluster distribution.

Our result for the exponent θ agrees with the (less accurate) value of Gaunt and Brak (1985) but disagrees with that of Cambier and Nauenberg (1986). These authors find that the FB theory holds in two dimensions with values for the critical exponents different from the ones computed here. In particular, they find $\theta = 2.4 \pm 0.2$. This value is totally excluded by our data. We think that their analysis in terms of scaling with temperature is hampered by finite-size effects and what they are computing are indeed effective exponents.

5. Conclusions

We have analysed by Monte Carlo methods the scaling ansatz (2.3) concerning the critical behaviour of the equilibrium cluster distribution of the two-dimensional Ising model in zero magnetic field. Our results show that (2.3) indeed holds but the values of the critical exponents τ and s are different from the ones predicted by existing theories. A new phenomenological theory has been developed by incorporating into the standard Fisher-Binder model a sum rule which is deduced in the framework of the Bruce-Wallace theory.

The discrepancy of the BW theory with the simulation results can be quantitatively measured as the difference between the observed and predicted values of the exponent y' in equations (4.11). While BW predict $y'_{BW} = \frac{30}{31}$, the observed value is $y' = 0.9579(49)$, the difference being $1 - y'/y'_{BW} = 1\%$. This discrepancy can be understood by the fact that the picture of the critical configurations which form the basis of the BW theory rests on the smallness of the parameter $\Psi_0 \equiv \beta/2\nu$; in two dimensions $\Psi_0 = 0.0625$ and the corrections are expected to be of order Ψ_0^2 which is the order of magnitude of the difference between y'_{BW} and y' observed.

The effect of the possible presence of the correction to scaling terms has been thoroughly investigated. The surprising conclusion is that these terms are of very little numerical importance for the second moment of the cluster distribution function (an expression for $p_2(L)$ without correction to scaling terms reproduces the exact values for $L = 1, 2, 3, 4$ with an error of less than 1%). This does not seem to be the case when analysing critical behaviour with the help of series expansions; Gaunt and Brak (1985) showed that, taking into account the correction to scaling terms, the value for the exponent θ is reduced by 2%. Our method deals with very large clusters and the phenomenon of nested clusters (which is indeed fundamental in the renormalisation group approach of BW) is fully considered by the cluster distribution observed in the simulation.

Finally, we want to emphasise the utility of the Monte Carlo method (when combined with a very fast updating algorithm) to extract very accurate results for the critical exponents. An extension of our work which is being considered is to study the critical exponents and critical densities for percolation phenomena in two and three dimensions.

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