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1984 J. Phys. A: Math. Gen. 17 1683

(http://iopscience.iop.org/0305-4470/17/8/024)

J. Phys. A: Math. Gen. **17** (1984) 1683–1701. Printed in Great Britain

Monte Carlo and series study of corrections to scaling in two-dimensional percolation

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Received 19 July 1983, in final form 19 December 1983

Abstract. Corrections to scaling for percolation cluster numbers in two dimensions are studied by Monte Carlo simulations of very large systems (up to 17×10^9 lattice sites) and by series analysis. Both series and Monte Carlo work suggests that the value of the correction-to-scaling exponent is slightly lower at the percolation threshold than away from it. Moreover, the corrections to scaling observed at p_c ($\Omega\cong0.64$) might be due to the mixing of scaling fields rather than to the irrelevant scaling fields. The Monte Carlo results are compatible with finite-size scaling, and finite-size scaling corrections are estimated. Technical problems associated with Monte Carlo simulation of very large systems are discussed in an appendix.

1. Introduction

The leading critical behaviour of two-dimensional percolation clusters is reasonably well understood (Stauffer 1979, Essam 1980). What are the corrections to those leading terms if one is close but not too close to the critical point? For percolation, there is no clear answer to this question (see, e.g., the recent review, Adler *et al* 1983).

The corrections to scaling for percolation cluster numbers in two dimensions have previously been studied using the Monte Carlo method by Hoshen *et al* (1979) and Nakanishi and Stanley (1980, 1981) for relatively small systems: triangular site percolation on (4000×4000) lattices and square bond percolation with (2000×2000) sites respectively. Hoshen *et al* (1979) studied the corrections to scaling only at the percolation threshold p_c and gave the value of the correction-to-scaling exponent $\Omega=0.67\pm0.1$. Nakanshi and Stanley (1980, 1981) estimated the correction-to-scaling exponent as $\Omega=0.6$–1.0.

In this paper we use very large systems (up to 17×10^9 sites), hoping that this approach will reduce the finite-size effects and therefore give more accurate estimates for Ω and a more complete picture of the scaling functions. For smaller lattices, Hoshen *et al* (1979) combined series and Monte Carlo data to estimate Ω. Here we want to rely only on Monte Carlo data for cluster sizes beyond those investigated by series.

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|| Supported in part by grants from NSF, ONR and ARO.

The previous works concentrated on testing the two-exponent scaling hypothesis of Stauffer (1975)

$$n_s(p) = s^{-\tau} f_0(z), \qquad z = (p_c - p)s^{\sigma}, \tag{1}$$

where $\tau = 2 + 1/\delta$, $\sigma = 1/\beta\delta$ and $n_s(p)$ is the average number of clusters per site of size s; we use standard notation for p, δ, and ν (Stauffer 1979). The corrections to scaling for percolation cluster numbers were introduced by Hoshen *et al* (1979) in the form

$$n_s(p) = s^{-\tau}(f_0(z) + s^{-\Omega} f_1(z)), \tag{2}$$

with the correction-to-scaling function $f_1(z)$ and the leading correction-to-scaling exponent Ω.

The purpose of this paper is to make a much more accurate estimate of the leading correction terms. We find that our data cannot distinguish between correction terms with slightly different Ω. Therefore, we estimate an *effective* correction-to-scaling exponent, and also an effective correction-to-scaling function $f_1(z)$. As a by-product, we obtain a more accurate estimate of the leading scaling function $f_0(z)$. We also find that there are indications from the series analysis of the corrections to scaling (Margolina *et al* 1982) that the value of Ω is not the same at the percolation threshold p_c as slightly below it. Therefore, we estimate Ω from Monte Carlo simulations not only at p_c but also away from it.

Our Monte Carlo data are compatible with finite-size scaling and we estimate the finite-size corrections along with the corrections to scaling. We make an attempt to reconcile our series and Monte Carlo data and explain why the Monte Carlo estimate of Ω is presumably closer to the 'true' value of Ω which might be due to the nonlinear scaling fields (Aharony and Fisher 1983).

The paper is organised as follows. In § 2 we present our Monte Carlo analysis at p_c and discuss the advantages of analysing extremely large systems for studying the corrections to scaling. In § 3 we present results for concentration p slightly below and above p_c. In § 4 we present calculations of the scaling functions $f_0(z)$, $f_1(z)$ defined in (2). In § 5 we compare series and Monte Carlo results and try to reconcile them. In § 6 we give our finite-size scaling analysis and discuss our choice of boundary conditions. In appendix 1 we give the details of our Monte Carlo simulations of large systems and various forms of random number generators used, while appendix 2 discusses subtleties of the Aharony–Fisher argument when applied to percolation.

2. Calculations at p_c

2.1. The advantages of large systems

Our results at p_c are based on the Monte Carlo study of the triangular lattices of sizes $L \times L$ with $L = 7000$, 10 000, 12 000, 17 000, 35 000, 50 000, 70 000, 95 000 and 130 000. The Monte Carlo algorithm was originally proposed by Hoshen and Kopelman (1976); additional technical problems arising from the analysis of very large systems are described in appendix 1.

We combine our cluster numbers n_s in bins in order to simplify the analysis and to reduce statistical fluctuations. We choose bins of exponentially increasing size, $2^i \leqslant s < 2^{i+1}$, $i = 0, 1, 2, \ldots$. The choice of bins with a width half as large, led to oscillations in our data. We use free boundary conditions, and take the conjectured

'exact' values of the leading exponents $\sigma = 36/91$; $\tau = 187/91$ (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980 and Nienhuis 1982).

The Monte Carlo data obtained for the number of isolated sites from our very large systems at p_c shows agreement to within 0.01% of the exact results comparing to 0.3% of Hoshen *et al* (1979) as shown in table 1. Our result $G = 0.017\,630 \pm 0.000\,02$ for the total number of clusters (normalised per site) disagrees significantly with the series estimate $G = 0.0168 \pm 0.0002$ (Domb and Pearce 1976).

The advantages of the very large systems for analysis of corrections to scaling are clear from figure 1, which shows the partial sums

$$N_s = s^{\tau-1} \sum_{s' \geqslant s} n_{s'}. \tag{3}$$

Table 1. The total number of clusters, $\Sigma_{s'} n_{s'}$, and the number of isolated sites, n_1, for various system sizes $L \times L$ at $p = p_c = \frac{1}{2}$ for the triangular lattice. The data for $L = 4000$ are taken from Hoshen *et al* (1979) and are based on 19 realisations. Data for $L = 12\,000$, 50 000, 70 000 are based on two realisations, while the remaining data are based on one realisation only. Here $\varepsilon = (n_1 - 1/128)/n_1$ is the relative deviation from the exact result: $n_1 = p_c(1-p_c)^6 = 1/128$.

L	$L^2 n_1$	ε	$\Sigma_s n_s$
4000	125 376	0.3%	—
7000	383 609	0.2%	0.017 701
12 000	1 125 104	0.09%	0.017 656
17 000	2 260 752	0.13%	0.017 657
35 000	9 573 663	0.035%	0.017 632
50 000	19 532 417	0.006%	0.017 631
70 000	38 284 057	0.007%	0.017 629
95 000	70 509 448	0.002%	0.017 630
130 000	132 035 615	0.003%	0.017 632

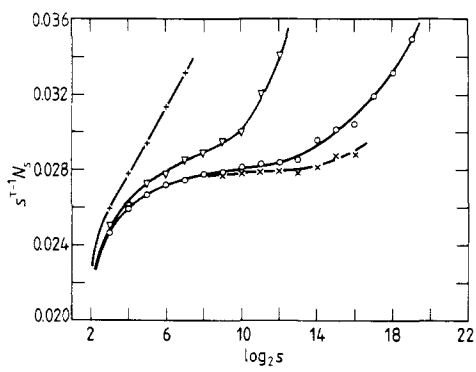

Figure 1. Dependence on $\log_2 s$ of partial sums $s^{\tau-1} \Sigma_{s' \geqslant s} n_s(p_c)$, obtained by Monte Carlo simulations for a $L \times L$ triangular lattice, for a sequence of increasing values of L: 1000 (+); 4000 (∇), 70 000 ($\bigcirc$) and 130 000 ($\times$). The points for $L = 4000$ are from Hoshen *et al* (1979).

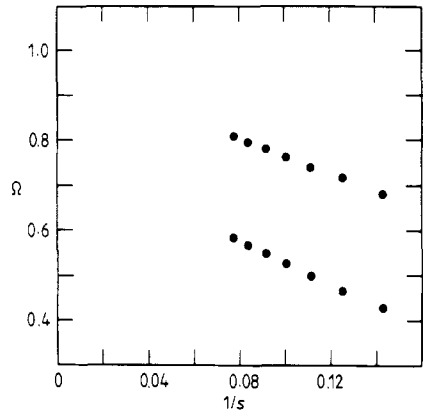

Figure 2. The correction-to-scaling exponents Ω calculated from three consecutive points via equation (5) are plotted against reciprocal central size $1/s$ at p_c (lower curve) and at p_{max} (upper curve) for triangular site percolation. The intercepts at $y_s = 0$ give our estimates, $\Omega(z = 0) = 0.8 \pm 0.1$ and $\Omega(z_{max}) = 0.98 \pm 0.1$.

The sum in (3) includes *all* clusters larger than $s = 2^i$ ($i = 0, 1, 2, \ldots$) in order to reduce the statistical error and avoid the problems inherent in the binning procedure. As described in Hoshen *et al* (1979) in the region of large s and at $p = p_c$ where the simple power law (1) is valid, we should observe a plateau for N_s: all partial sums would equal the same constant $f_0(0)/(\tau - 1)$ if the sums were replaced by integrals. In figure 1 we compare the results for relatively small systems with our results for very large systems. It is seen very clearly that there is almost no plateau for smaller systems while for very large systems we definitely observe a plateau, within the statistical error, for cluster sizes from about $s = 2^9$ to 2^{12}. The plateau flattens for larger systems, and the starting point of the 'overcounting' of smaller clusters on the right-hand side due to our free boundary conditions, moves to larger s for larger systems. The deviations for large s from the plateau value are thus due to the finite-size effects, confirming a speculation of Hoshen *et al* (1979). Unfortunately, for smaller systems the finite-size effects enter already for small cluster sizes of about $s = 2^5$–2^7. Therefore, an analysis providing more accurate information about the behaviour of scaling functions for larger cluster sizes needs larger system sizes than those used earlier. The somewhat erratic behaviour at large s prevents a detailed finite-size scaling description of the increase beyond the plateau.

The deviations from the 'plateau value' on the left side of figure 1 are due to the corrections to scaling, as noted by Hoshen *et al* (1979). For small s one observes drastic deviations of the results for the smaller systems from each other, while our results for $L = 35\,000$, $50\,000$, $70\,000$, $95\,000$ and $130\,000$ practically overlap for cluster sizes $s = 2^4$–2^8. Thus, this is the range of cluster sizes where the leading correction to scaling function $f_1(z)$ can be accurately measured. This is seen more clearly if the deviations of the partial sums from the averaged plateau value are plotted versus $s^{-\Omega}$ for the correction-to-scaling exponent Ω of about 0.6–0.7. In the range of cluster sizes $s = 2^4$–2^8 we observe approximately linear behaviour of these deviations. Therefore, from now on we concentrate on this range of cluster sizes for the analysis of the corrections to scaling. For larger systems, however, e.g., $L = 95\,000$ and $130\,000$, we could reach for larger $s = 2^9$–2^{12} when analysing the corrections to scaling.

2.2. *Monte Carlo analysis*

The value of Ω is estimated by linearly fitting the partial sums N_s of (3) to $s^{-\Omega}$ for various ranges of s, e.g. $s = 2^4$–2^8. This estimated values of Ω seem to depend on the chosen range of s as shown in table 2. We have also used several other methods to estimate Ω: e.g., linear fits to the log–log plot of the $(s^{\tau-1} \Sigma_{s' \geq s} n_{s'} - q_0/(\tau - 1))$ against s with q_0 being varied to achieve the best linearity. However, all methods gave results similar to those of table 2 in magnitudes and in scatter.

For larger systems, where we are able to analyse larger clusters, Ω tends to decrease. However our run for $L = 130\,000$ gives an unexpectedly higher value of Ω. Our estimate is $\Omega = 0.64 \pm 0.08$. However, the statistical error for a particular fit (table 2) is usually much smaller (about 0.02–0.03). Our finite-size scaling analysis gives an estimate of Ω somewhat higher (about 0.66). The finite-size scaling analysis and the discussion of free boundary conditions are presented in § 5. For a reader who wants to make his own analysis, table 3 gives our raw data for $L = 95\,000$. The relative statistical error for cluster numbers N_s is about $1/\sqrt{N_s}$ according to the rigorous results of Coniglio *et al* (1979).

Table 2. The values of Ω estimated by linear fitting of the partial sums $s^{\tau-1}\Sigma_{s'\geq s} n_{s'}$ to $s^{-\Omega}$ for various lattice sizes L and ranges of s (the error bars shown are purely statistical). The values in square brackets are due to particularly bad fits, and the hyphens stand for unrealistic fits.

s	$L=35\,000$	$L=50\,000$	$L=70\,000$	$L=95\,000$	$L=130\,000$
16–512	0.60 ± 0.1	0.66 ± 0.03	0.64 ± 0.03	0.64 ± 0.01	0.67 ± 0.02
8–512	—	0.65 ± 0.05	0.66 ± 0.02	0.65 ± 0.02	0.66 ± 0.03
16–1024	0.59 ± 0.07	0.70 ± 0.05	0.58 ± 0.07	0.64 ± 0.02	0.68 ± 0.03
8–1024	—	0.67 ± 0.02	0.62 ± 0.04	0.64 ± 0.02	0.66 ± 0.03
16–2048	—	$[0.57\pm0.10]$	$[0.50\pm0.10]$	0.63 ± 0.02	0.68 ± 0.02
8–2048	—	$[0.56\pm0.10]$	$[0.61\pm0.10]$	0.64 ± 0.03	0.67 ± 0.03
16–4096	—	—	—	0.60 ± 0.02	0.67 ± 0.03
8–4096	—	—	—	0.62 ± 0.03	0.66 ± 0.04
16–8192	—	—	—	0.58 ± 0.03	0.65 ± 0.04
8–8192	—	—	—	0.61 ± 0.03	0.65 ± 0.04
average	0.60 ± 0.10	0.67 ± 0.05	0.63 ± 0.07	0.64 ± 0.03	0.67 ± 0.04

Table 3. Cluster numbers $N_s = L^2 \times n_s$ and partial sums $s^{\tau-1}\Sigma_{s'} n_{s'}$ for triangular lattice of size $L=95\,000$ at $p=p_c=\frac{1}{2}$.

s	N_s	$s^{\tau-1}\Sigma_{s'} n_{s'}$
1	70 509 448	0.017 630
2–4	40 775 040	0.020 397
4–8	22 993 658	0.022 876
8–16	12 296 831	0.024 678
16–32	6322 749	0.025 884
32–64	3168 306	0.026 657
64–128	1563 389	0.027 148
128–256	763 790	0.027 456
256–512	371 268	0.027 661
512–1024	179 822	0.027 798
1024–2048	86 785	0.027 893
2048–4096	42 036	0.028 010
4096–8192	20 224	0.028 064
8192–16 384	9752	0.028 188
16 384–32 768	4731	0.028 391
32 768–65 536	2267	0.028 574

The 'plateau value' we get from our results is about $f_0(0)=0.0295$ and is in good agreement with the plateau value given by Hoshen *et al* (1979): $f_0(0)=0.03$. The ratio of $|f_1(0)|/[f_0(0)]$ is less than unity, which is lower than the estimate of Hoshen *et al* (1979) $|f_1(0)|/[f_0(0)]=1.19$ but it is dependent on the estimate of Ω chosen.

3. Results for $p \neq p_c$

We have also made Monte Carlo simulations for concentration p slightly above and below p_c within the scaling region

$$|p_c - p| \sim s^{-\sigma}, \tag{4}$$

to estimate the corrections to scaling away from p_c. Our main interest here is the value $p = p_{max}(s)$ where $n_s(p)$ has a maximum as a function of p at fixed s. The corresponding value of the scaling variable $z_{max} \simeq (p_c - p_{max})s^{\sigma}$ was found by Hoshen *et al* (1979) to be $z_{max} \simeq 0.44$. We want to test more carefully the previous result of series analysis (Margolina *et al* 1983) which seemed to indicate that $\Omega(z_{max}) > \Omega(0)$.

3.1. Series analysis

We use the following ratio-like method in our series analysis. Within the scaling region (4), the scaling assumption (2) implies

$$s^{\tau} n_s(p) = f_0(z) + s^{-\Omega(z)} f_1(z). \tag{5}$$

Here we denote the effective dependence of Ω on z as $\Omega(z)$. Actually, the impression that Ω varies continuously with z is likely to be an artifact of a numerical method. We expect one value of Ω at $p = p_c$ and another at fixed $p < p_c$, corresponding to the crossover between percolation and lattice animals (see, e.g., Family and Coniglio 1980). However, the essence of the assumed two-exponent scaling hypothesis (2) is that for all data within the scaling region (4) ($z = \text{const}$), we automatically preserve the same (percolation) type of critical behaviour. Therefore, throughout our analysis we keep the same values of the critical exponents σ and τ. We take again $\tau = 187/91$ and try to estimate $\Omega(z)$ for $z = 0$ and $z = z_{max}$ from the series expansions of $n_s(p)$ (Sykes *et al* 1976, Margolina *et al* 1983).

If we treat $n_s(p)$ calculated from the series expansions as 'experimental' points and then make three-point fits with equation (5), we can calculate the value of Ω_s for each set of the three consecutive values of s. Then we plot these three-point exponents versus the reciprocal central size s and get the estimate of the asymptotic exponent Ω as an intercept for $1/s \to 0$. We carry out this analysis for $p = p_c$ and $p = p_{max}$. We note that the advantage of this method is that the values of $n_s(p_c)$ are exact for the lattice where p_c is known exactly and the values of p_{max} for each fixed s can be calculated very accurately from the series expansion polynomials.

The results of applying this method to triangular and square-site problems are shown in figure 2. The values obtained are: for triangular lattice $\Omega(0) = 0{\cdot}8 \pm 0.1$; $\Omega(z_{max}) = 0.98 \pm 0.1$; for square lattice $\Omega(0) = 0.75 \pm 0.1$; $\Omega(z_{max}) = 1.0 \pm 0.1$. The maximum error bar of this method is about 15% and is of the same order as the difference between the two values of Ω.

Our results for the triangular lattice do not change much when we apply our method to analyse the additional fifteenth term in the series expansion (Margolina *et al* 1983); on the other hand, the same fifteenth term as analysed by Adler (private communication) lowers the previous estimate of Adler *et al* (1983) of $\Omega \simeq 0.66$ to $\Omega \simeq 0.64$. For further analysis one can take intermediate values of p so that $p_c - p = \alpha(p_c - p_{max})$ with $0 < \alpha < 1$. The values of p chosen this way ensure that p is within the scaling region (4). As a result we conclude that the effective $\Omega(z)$ is a smooth increasing function of z, i.e., the effective Ω gets larger when p moves away from p_c. The range of Ω is 0.7–1.0. Other two-dimensional lattices show indications of a similar behaviour of $\Omega(z)$ though less sharply. We tried to carry out the same analysis for three-dimensional problems using the value of $\tau \simeq 2.21$, $\sigma \simeq 0.46$ and $p_c = 0.3117$ from Gaunt and Sykes (1983). Only the FCC lattice shows the same effect for $\Omega(z)$, namely Ω varies in the range of 0.8–1.1 for different p within the scaling region. Other series expansion

polynomials in higher dimensions are not long enough to show clear asymptotic behaviour.

3.2. Monte Carlo analysis at $p \neq p_c$

Thus, our preliminary series analysis indicates some difference between the estimated values of $\Omega(0)$ and $\Omega(z_{max})$. This calls for more accurate numerical work that can treat cluster sizes far beyond those available to series expansions. Since the value of p_{max} is actually a function of cluster size s, several runs for different fixed concentrations p are necessary to obtain the scaling picture away from p_c ($z \neq 0$) by Monte Carlo simulations. Therefore, with the same amount of computer time we do not get the same accuracy as at p_c. If we choose one of the bins within the chosen range of cluster sizes $2^4 \leqslant s < 2^8$ as a starting point, then we obtain the starting concentration value p_s from

$$(p_c - p_s) s_{average}^{\sigma} = z_{max}. \tag{6a}$$

For example, if $i = 5$ ($2^5 \leqslant s < 2^6$), then $s_{average} = (32 \times 64)^{1/2} = 45$. Taking $z_{max} = 0.44$ from Hoshen *et al* (1979) we therefore obtain the starting concentration value $p_s \simeq 0.4$. In order to preserve the value of z_{max} throughout the analysis we then shift to the neighbouring bins s^* changing the concentration values p_s to p_s^* according to

$$(p_c - p_s) s_{average}^{\sigma} = (p_c - p_s^*) s_{average}^{*\sigma}. \tag{6b}$$

We performed two realisations at $p < p_c$ for each of the five concentrations p_s obtained this way and one run at $p > p_c$ ($z < 0$) for each of the six concentrations p symmetrical to those of $p < p_c$) for the triangular lattice with $L = 35\,000$ and five runs for five concentrations $p < p_c$ for the triangular lattice $L = 70\,000$. The partial sums are no longer useful at $z \neq 0$, since one needs many realisations for each fixed z to get cluster numbers $n_s(z)$, tabulated by (s^*, p_s^*), as shown in table 4.

It seems reasonable, therefore, to take the sums

$$Q(i) = s_{average}^{\tau - 1} \sum_{s'=2^i}^{2^{i+1}-1} n_{s'} \tag{7}$$

(where $s_{average} = 2^{i+1/2}$) over each bin i instead of partial sums, and fit these sums to $s^{-\Omega(z)}$ for each z according to the scaling assumption (5). As a by-product of this

Table 4. Table of cluster numbers $N_s(p) = L^2 \times n_s(p)$ for lattice size $L = 70\,000$ at five concentrations $p < p_c$: $p_4 = 0.36\,845$, $p_5 = 0.40\,000$, $p_6 = 0.42\,398$, $p_7 = 0.44\,214$, $p_8 = 0.45\,607$ and corresponding bins $s = 2^i - 2^{i+1}$ with $i = 3, 4, 5, 6, 7, 8, 9$ (the value of z_{max} corresponds, e.g., to concentration p_4 and bin $i = 4$). We read off the numbers $n_s(p)$ for fixed p and different s from a line, while the values of $n_s(z)$ for fixed z and different s we read off from a diagonal.

	$i=3$	4	5	6	7	8	9
p_4	34 299 278	18 476 117	7287 614	1534 112	—	—	—
p_5	27 672 296	16 869 613	8980 802	3532 314	750 446	—	—
p_6	—	13 716 188	8228 306	4343 508	1707 118	363 161	—
p_7	—	—	6721 532	3990 190	2097 008	823 325	174 069
p_8	—	—	—	3268 279	1929 824	1012 262	395 004

linear fitting one finds, from a slope and an intercept, the scaling functions $f_1(z)$ and $f_0(z)$ for each trial value of $\Omega(z)$. Our best estimates of the $\Omega(z_{max})$ are given in table 5 for different ranges of s. Note that the maximum range of s available at $z = z_{max}$ is from 2^4–2^8 corresponding to our choice of five fixed concentrations p. Each run for $L = 70\,000$ takes about five hours on an IBM 370/168, so one chooses the well established range of $s = 2^4$–2^8 rather than making additional test runs.

Table 5. The values of Ω estimated by linearly fitting of the sums $s_{average}^{\tau-1} \Sigma_{bin} n_s(z)$ to $s^{-\Omega(z)}$ for lattice sizes $L = 35\,000$, $70\,000$ and various ranges of s within the chosen range $s = 2^4$–2^8 at $z = z_{max}$ compared to the values of Ω at $p_c(z = 0)$ estimated by the same method. The values in brackets are due to particularly bad fits and the dashes stand for unrealistic fits.

	$z = z_{max}$		$z = 0$	
s	$L = 35\,000$	$L = 70\,000$	$L = 35\,000$	$L = 70\,000$
16–512	0.78 ± 0.03	0.73 ± 0.03	0.65 ± 0.03	0.72 ± 0.03
32–512	0.74 ± 0.02	(0.50 ± 0.10)	—	0.72 ± 0.04
16–256	0.79 ± 0.03	(0.89 ± 0.10)	0.61 ± 0.07	0.72 ± 0.04
32–256	0.74 ± 0.04	(0.65 ± 0.10)	—	0.69 ± 0.05
16–128	(0.81 ± 0.10)	—	—	0.72 ± 0.03
average	0.77	0.69	0.63	0.71

3.3. Results

The overall average estimate of Ω at z_{max} is $\Omega_{max} = 0.75$ which is, indeed, slightly higher than at the percolation threshold. But there are several uncertainties here. First, for the larger lattice $L = 70\,000$ we get the average value of Ω smaller than for the one with $L = 35\,000$, and we hope that the results for larger lattices are more reliable. Second, we compare in table 5 our results of fitting of the sums (7) at z_{max} and of fitting of the same sums (7) at $z = 0$ (as opposed to the fitting of partial sums). The fitting of sums (7) seems to give on the average the value of Ω slightly higher, even at p_c. The reasons for that might be inherent in the binning procedure, but then it seems more consistent not to compare our results at z_{max} to those at $z = 0$ obtained by fitting the partial sums (3) but rather to those at $z = 0$ obtained by fitting the sums (7). Comparisons such as that in table 5 lead to consider the two estimates of Ω to be too close to be distinguished within the accuracy of our method.

Another question here is how to estimate the error bar: is it larger or smaller than at p_c? Our fitting procedure seems not to be as reliable as the fitting of partial sums. On the other hand, the fluctuations of cluster numbers $n_s(p)$ at z_{max} might be smaller than the critical fluctuations at p_c (Jan and Stauffer 1982). Therefore it is not clear what the confidence limits are of the estimated value of $\Omega(z_{max})$, and, therefore, the question about the existence of the dependence of $\Omega(z)$ is still open. Our best fit for $z < 0$ ($p > p_c$) was not for $z = -z_{max}$ but for $z = -z_{max}2^{-\sigma}$: $\Omega \simeq 0.76$ (based on one run for $L = 35\,000$). Other fits were not as good but the average value of Ω is about 0.7 for the chosen range of cluster sizes and the values of $f_0(z)$, $f_1(z)$ obtained for each Ω_{trial} are consistent with each other.

The conclusion of this analysis is that there are two possibilities.

(i) One possibility is to accept the apparent difference between $\Omega(z_{max})$ and $\Omega(0)$ and to search for a reason for it. A tentative explanation is presented in § 5. We will also compare our series estimates with our Monte Carlo estimates of Ω, which tend to be lower, and discuss what might be the reasons for this discrepancy.

(ii) A second possibility is to keep the standard form of the correction term (2) and try to fit the data into the unified picture with the average Ω of about 0.7. We attempt to do so in § 4.

4. The scaling functions $f_0(z)$, $f_1(z)$

Let us assume now that Ω has the same value at all z of about 0.7 (the average over all our estimates) or about 0.6 (see § 5 for a possible justification of the value of $\Omega \cong 0.6$) and try to fit all our data at, above and below p_c on the scaling assumption (5). Thus, we determined $f_0(z)$ and $f_1(z)$ for different z as the intercept and slope, respectively, of a linear fit of $s^{\tau-1}\Sigma_{bin}\, n_s(p)$ to $s^{-\Omega}$. Note that most of the values of $f_0(z)$, $f_1(z)$ shown below are obtained from fits far from the best since it is hard to fit all our data with one Ω value as explained in § 3. This circumstance should not affect much the form of the leading scaling function $f_0(z)$ which is not sensitive to the choice of Ω and which appears to be very similar to the one found by Hoshen *et al* (1979). Unfortunately, the value of Ω chosen affects the form of the correction-to-scaling function $f_1(z)$ (sometimes beyond the shown statistical error bars). The result of our attempt to fit all our data with only one Ω value is shown in figure 3. From this picture one may see that while $\ln f_0(z)$ is a smooth parabola–like function which has a maximum at $z = z_{max}$, the function $\ln f_1(z)$ oscillates for $z < 0$ ($p < p_c$). But within the error bars it might also be presented as a smooth parabola-like curve with the maximum at z slightly below z_{max}. While at p_c the functions $f_0(z)$ and $f_1(z)$ are not much different, at $z = z_{max}$, $f_1(z)$ is about five times smaller than $f_0(z)$. Above p_c the correction function $f_1(z)$ seems to decay slower than the leading function $f_0(z)$. If this trend continues for larger $|z|$ the contribution from the correction term would be, for very large and rare clusters, larger than that from the leading term. The ratio $f_0(z_{max})/f_0(0)$ obtained is about 4.9 which is in good agreement with Hoshen *et al* (1979) $f_0(z_{max})/f_0(0) = 4.9 \pm 0.1$, and Djordjevic *et al* (1982) $f_0(z_{max})/f_0(0) = 4.8$–$5.1$.

5. Discussion

5.1. Three discrepancies

In this section we will make an attempt to reconcile all the numerous series and Monte Carlo results for the correction-to-scaling exponent Ω in two dimensions (for the detailed review of estimated and conjectured values of Ω see Adler *et al* 1983). Our Monte Carlo result at the percolation threshold p_c (see § 2) $\Omega = 0.64 \pm 0.08$ is the lowest of all the existing numerical estimates of Ω. Our result is in good agreement with the estimate of Hoshen *et al* (1979), $\Omega = 0.67 \pm 0.1$. However, we never found Ω to be as high as the central value from previous series analysis $\Omega = 0.75 \pm 0.05$ (Gaunt and Sykes 1976) or from our own series analysis $\Omega = 0.8 \pm 0.1$ (see § 3). On the other hand, a recent result of a different type of series analysis (Adler *et al* 1983) gives a direct estimate of $\Omega = 0.66 \pm 0.07$ (which is in very good agreement with our Monte

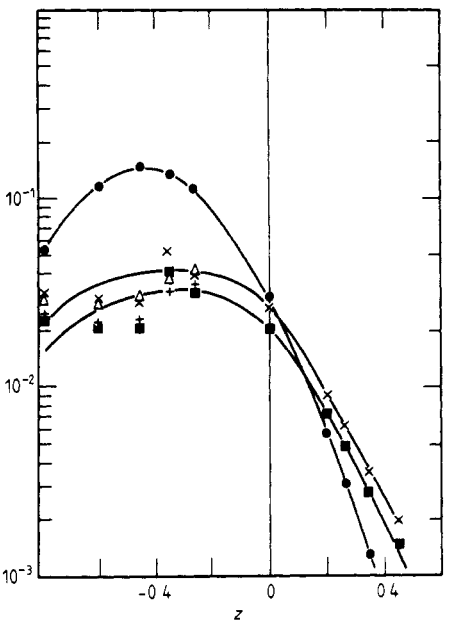

Figure 3. Scaling function $f_0(z)$ (top curve) and 'correction-to-scaling function' $-f_1(z)$ (lower two curves) obtained by Monte Carlo simulations on triangular lattices with 2.5×10^9 sites and 5×10^9 sites. Two trial values of Ω are used in calculating these functions, $\Omega=0.6$ (■ and +, corresponding to the two runs for a lattice with 2.5×10^9, sites and one run for a lattice with 5×10^9 sites, respectively) and $\Omega=0.7$ (× and △, similarly). The function $f_0(z)$ was not visibly different for the two cases, so only one full curve is shown.

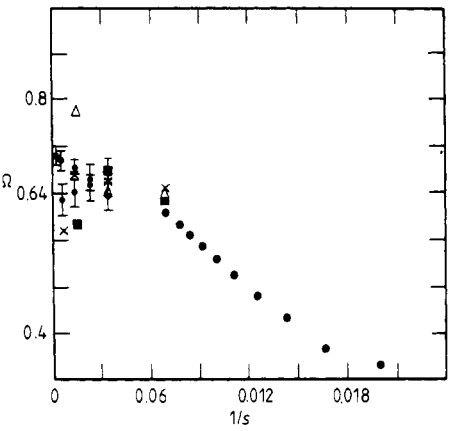

Figure 4. The same data as figure 2, at $p=p_c$, continued to smaller values of $1/s$ by treating Monte Carlo data 'as if' these data were obtained from series. The symbols △, □, × correspond to the values of Ω obtained from three consecutive points for $L=50\,000$, $70\,000$ and $95\,000$ respectively. The larger and smaller error bars are obtained from fitting over the extended ranges of s for $L=95\,000$ and $130\,000$ respectively. The x-axis is $(s_{\text{average}})^{-1}$ for this case, where s_{average} is the geometric mean of the lowest and highest bins used (e.g., $s_{\text{average}}=2^7$ for the data in the range 2^4–2^{10}).

Carlo analysis) and an indirect one (from an estimate of Δ_1) of $\Omega\simeq0.48$. There are thus three types of discrepancy: our Monte Carlo results differ from our series results (series results are higher), our series results differ from the Adler *et al* (1983) series results, and the Adler *et al* (1983) direct estimate differs from their own indirect estimate using Δ_1 (the exponent for $p-p_c$ in the leading correction factor).

5.2. The 'true' Ω

One wonders if the true value of Ω is somewhere in between the lowest and highest estimates (approximately 0.7) or if the very slight trend towards lower Ω shown by including clusters of much larger sizes leads to approximately 0.6. Still another possibility, as suggested by our estimates of Ω at $p\neq p_c$ and by Adler *et al* (1983), is that two or more exponents (e.g. $\Omega\simeq0.6$ and $\Omega\simeq0.7$) might compete at p_c and at $p\neq p_c$. The value $\Omega\simeq0.6$ might be justified by applying the Aharony–Fisher concept of the corrections to scaling due to the nonlinear scaling fields to percolation. This application would imply already, in linear order, a mixing of temperature-like and field-like scaling variables (p_c-p) and h (or $1/s$, since it is known (Stanley and Coniglio 1983) that

the scaling power $y_h = -y_s$). This linear mixing, however, would not be allowed if the symmetry of the q-state Potts model were to be respected (see appendix 2). If $q = 1$ Potts model (percolation) would prove to be an exception, one would replace $\varepsilon = p_c - p$ by the scaling field $g_p = [\varepsilon + \varepsilon^2 + 1/s + \ldots]$ and $1/s$ by the scaling field $g_s = [1/s + 1/s^2 + \varepsilon/s + \ldots]$. As $p = p_c$ ($\varepsilon = 0$), we find on expanding the leading term of (2)

$$\begin{aligned} n_s(p_c) &= g_s^{\tau} f_0(g_p/g_s^{\sigma}) = s^{-\tau} f_0(s^{-(1-\sigma)}) + \ldots \\ &= s^{-\tau}(f_0(0) + s^{-(1-\sigma)} f_0'(0) + \ldots). \end{aligned} \tag{8}$$

Hence the leading correction-to-scaling exponent $\Omega = 1 - \sigma = 1 - 1/\beta\delta \simeq 0.6$. One would then also find many other correction terms at $p \neq p_c$ (for fixed $z = (p_c - p)s^{\sigma} \neq 0$) with various values of Ω close to each other. These values arise from the various terms in g_s and g_p since within the scaling region (4) $\varepsilon \sim s^{-\sigma}$, e.g., at $z = z_{\max}$ expanding $f_0(z)$ around its maximum value one finds after some algebra that there are *three* values of $\Omega < 1$. I.e., in addition to the analytic $1/s$ correction, there are three possible non-analytic corrections with $\Omega = \sigma$, $1 - \sigma$ and 2σ. The competition between those terms with amplitudes depending on the scaled variable $z = (p_c - p)s^{\sigma}$ might account for the different effective values of the correction-to-scaling exponent Ω away from the percolation threshold p_c. But even apart from this tentative interpretation, the numerical data by themselves are not inconsistent with the existence of the correction term with $\Omega \simeq 0.6$.

5.3. *The 'effective' Ω*

There is a discrepancy between the results of the ratio-like type of series analysis used by Gaunt and Sykes (1976) and by us (which overestimate Ω) and the results of the method of Adler *et al* (1983) designed for studying the corrections to scaling. The reason for this discrepancy might be that the ratio-like methods (and also Monte Carlo analysis) pick up all the 'background' and therefore obtain an effective Ω (cf Greywall and Ahlers 1973).

The degree of 'background' effect may also explain another major discrepancy, that between ratio-like series analysis and our own Monte Carlo results. To see this, note that the effective Ω is defined at p_c as

$$\Omega_{\text{eff}} = -\log|(s^{\tau} n_s(p_c) - f_0(0))|/\log s \simeq \Omega + (f_2(0)/f_1(0))(\Omega_2 - \Omega)\bar{s}^{(\Omega - \Omega_2)}. \tag{9}$$

Here $f_2(0)$ is the amplitude of the next-to-the-leading correction term with the exponent $\Omega_2 > \Omega$; $\bar{s}$ is the value of s suitably averaged over the region of analysis. Let us compare now the values of Ω_{eff} one would get from series analysis ($\bar{s} \simeq 10$) and Monte Carlo analysis ($\bar{s} \simeq 100$ or even $\bar{s} \simeq 1000$ if one only takes into account larger clusters 2^9–2^{11}) if we had $\Omega = 1 - \sigma \simeq 0.6$ and $\Omega_2 = 1.0$ (assuming the next correction is analytic). Then Ω_{eff} becomes linear in $\bar{s}^{-\sigma}$ and one gets for series with $\bar{s} \simeq 10$: $\Omega_{\text{eff}} = 0.6 + (f_2(0)/f_1(0))0.16$ and for Monte Carlo $\Omega_{\text{eff}} = 0.6 + (f_2(0)/f_1(0))0.06$ for $\bar{s} \simeq 100$ or $\Omega_{\text{eff}} = 0.6 + (f_2(0)/f_1(0))0.03$ (for $\bar{s} \simeq 1000$). The correction will be positive if $f_2(0) < 0$ (since we know that $f_1(0) < 0$) and if $f_2(0)$ is of the order of $f_1(0)$ (similarly to $f_1(0)$ being of the order of $f(0)$ as seen in figure 3) this comparison might account for the discrepancy between our series and Monte Carlo results. This argument becomes weaker, though, if there exists an Ω_2 in between 0.6 and 1, e.g., $\Omega_2 \simeq 0.8$, but it still shows some difference between the effective Ω obtained by different methods.

On the other hand, Adler *et al* (1983) claim true exponents instead of effective ones, and try to distinguish between the two close values of Ω.

5.4. Attempt to reconcile series and Monte Carlo results

There is another way to understand the difference between our series and Monte Carlo data in one picture (see figure 4). The Monte Carlo data obtained for our largest systems with over 2×10^9 sites are good enough to be analysed as if they were series data (see the method in § 2), namely from three consecutive points (like $s=32$, 64, 128) we calculate the s-dependent Ω_s using (5) and then plot it against the reciprocal central value of s (e.g. 1/64 in the above example) together with the series results. Only for $s_{\text{central}}=16$ (meaning the fit for $s=8$, 16, 32) the Monte Carlo result is compatible with series results. But for $s>16$ the curve seems to show a maximum and then decreases to $\Omega\sim0.6$, or it flattens (as it is the case for our largest system of 17×10^9 sites) giving $\Omega\sim0.7$. One might also plot on the same picture the values of Ω fitted over different extended ranges of s (like $s=2^4$–2^8 or $s=2^5$–2^{11}) against the reciprocal average s of this range ($s=2^6$ or $s=2^8$ in the above example). There is, however, an ambiguity here since the average s is the same for ranges $s=2^4$–2^8 and $s=2^3$–2^9 but Ω usually are not. We show these fitted Ω only for the two largest lattices on figure 4 and, interestingly, the lattice with 9×10^9 shows a maximum while the lattice with 17×10^9 sites shows a flattening, if not monotonic, behaviour. Hence, the only conclusion we can draw from figure 4 is that the ratio-like series methods, which use only rather small s, *overestimate* Ω.

5.5. The two values of Ω

The last major discrepancy arises in the work of Adler *et al* (1983) where the estimates of Ω and Δ_1 were made independently and failed to reconcile via the relation (Nakanishi and Stanley 1980)

$$\Omega=\Delta_1/\beta\delta \tag{10}$$

(Δ_1 was found to be around 1.25, which gives $\Omega\simeq0.48$ as compared to the value of Ω found by the same authors: $\Omega\simeq0.59$–0.73). If one takes this discrepancy seriously† one might conclude that the reason why this lower exponent $\Omega\simeq0.48$ does not show in our analysis is that the amplitude of the corresponding correction term is very small. We could also speculate as follows. The estimate of Δ_1 was made from the analysis of the series expansions of susceptibility where the 'ghost-field' was set to zero ($h=0$). Therefore no Aharony–Fisher (1983) type correction was present, apart from a trivial analytic correction with $\Delta_1=1$. Hence one finds here the correction-to-scaling term due to the irrelevant field‡. But analysing the Monte Carlo and series data for percolation cluster numbers for $p=p_c$ and $h\neq0$ one should have observed both exponents: $\Omega\simeq0.6$ and $\Omega\simeq0.5$. Therefore, this gives one more reason to believe in lower values of the effective exponents as opposed to the higher ones.

† The quoted value of Δ is in agreement with that of Stauffer (1981) and was recently confirmed by Privman and Fisher (1983) by the study of the convergence properties of the phenomenological renormalisation data. However, Herrmann and Stauffer (1983) have arguments that in the type of data analysed by Stauffer (1981) the correction term is $L^{-1/\nu}\simeq L^{-0.75}$ which agrees well with the data and has nothing to do with the Δ_1 discussed.

‡ The value of $\Delta_1=1.25$, notably, is close to the value of Δ_1 for n-vector model in two dimensions (Le Guillou and Zinn-Justin 1980) and the corresponding value of Ω is relatively close to the value of $\sigma\simeq0.4$.

6. Finite-size scaling analysis

For our systems of finite (though very large) linear size L one might postulate, following Margolina *et al* (1982), a finite-size scaling hypothesis for large s, large L and p close to p_c

$$n_s(p) \simeq s^{-\tau} f(z, s^{1/D}L^{-1}) + s^{-\tau-\Omega} f_1(z, s^{1/D}L^{-1}), \tag{11}$$

where D is the fractal dimension (Stanley 1977, Stanley and Coniglio 1983), $1/D = \sigma\nu = 48/91$ is the mean cluster radius exponent, and $z = (p_c - p)s^{\sigma}$. For $s \ll L$ but still large (this is no problem for our very large systems) one can expand $n_s(p)$ in $s^{1/D}L^{-1}$ and leaving only the linear term one gets at p_c

$$n_s(p_c) \simeq s^{-\tau}(q_0 + q_1 s^{-\Omega} + q_L s^{1/D}L^{-1}), \tag{12}$$

where q_0, q_1, q_L are constants independent of s and L and the last term is the leading finite-size correction. This linear form of correction is suggested, in our case, by the choice of free boundary conditions. Thus, a fraction of large clusters is split into smaller clusters due to finite L. This leads to an overcounting of smaller clusters by an amount proportional to $s^{1/D}L^{-1}$ as discussed in § 2. Therefore, it seems plausible to consider the finite-size corrections linear in $s^{1/D}L^{-1}$ along with the corrections to scaling. Note that it is not clear whether the choice of the periodic boundary conditions would make things better but it would certainly cost more memory space (see Heermann and Stauffer 1980, Jan and Steinitz 1983). Periodic boundary conditions instead of free boundaries would reduce the finite-size effect for small clusters. But it is not clear whether they would have been useful for the 'plateau' cluster sizes we are interested in. Our data for the largest lattices (sizes larger than 2.5×10^9 sites) turn out to be compatible with finite-size scaling hypothesis (12) (see figure 5). We therefore make an attempt to fit our data including the finite-size corrections. Thus, for a given $\hat{q}_L$ a linear least-squares fit was made of the function $(N_s - \hat{q}_L s^{1/D}L^{-1})$ against $s^{-\Omega}$.

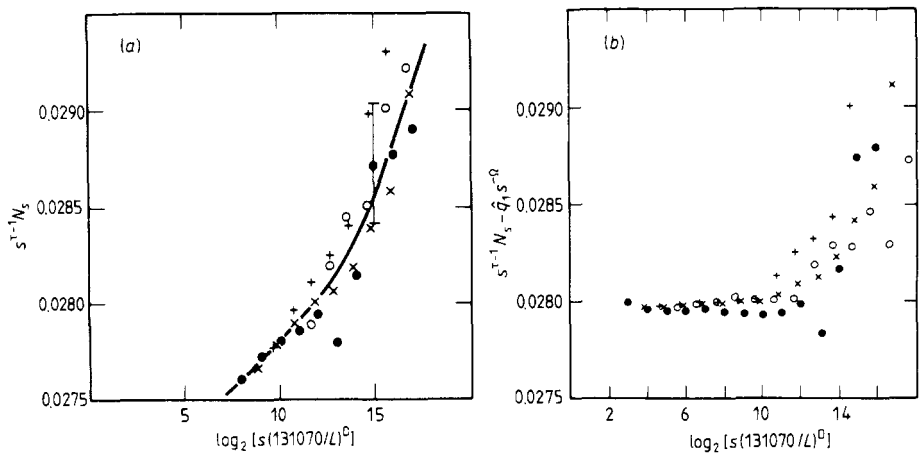

Figure 5. (*a*) Finite-size scaling plot showing the values of partial sums $s^{\tau-1}\Sigma_{s' \geq s} n_{s'}$ of equation (3) for various lattice sizes, $L = 50\,000$ (○), $70\,000$ (+), $95\,000$ (×) and $130\,000$ (●). The error bar shown is representative. For part (*b*), the y-axis is $s^{\tau-1}\Sigma_{s' \geq s} n_{s'} - \hat{q}_1 s^{-\Omega}$ where $\hat{q}_1 = 0.013$ and $\Omega = 0.66$ is estimated by a joint fit of the four largest lattices sizes.

The partial sums (3) for different s in the same computer run (same L) are not statistically independent, whereas those in different runs are. Hence we fit the data separately for each L as a function of parameter q_L and then select the value of Ω for which the total error becomes minimum. The total error is taken to be the mean square deviation for $L = 130\,000$ plus half of the mean-square deviation for $L = 95\,000$ plus quarter of the mean-square deviation for $L = 70\,000$. This minimum value is plotted in figure 6 against the chosen finite-size parameter q_L. It shows a minimum at about $q_L = 0.092 \pm 0.08$. The value of Ω obtained by this joint fit for $s = 2^3$–2^9 of our four largest lattice sizes increases our effective Ω to

$$\Omega = 0.66 \pm 0.03 \tag{13}$$

(the error bar is purely statistical). However, a larger error bar due to the unknown systematic errors would still not exclude the value of $\Omega \cong 0.6$†. The value obtained for $q_0 = 0.0294$ agrees with the plateau value for partial sums obtained in § 2 after the subtraction of the finite-size effect. For the partial sums one gets, finally, the scaling

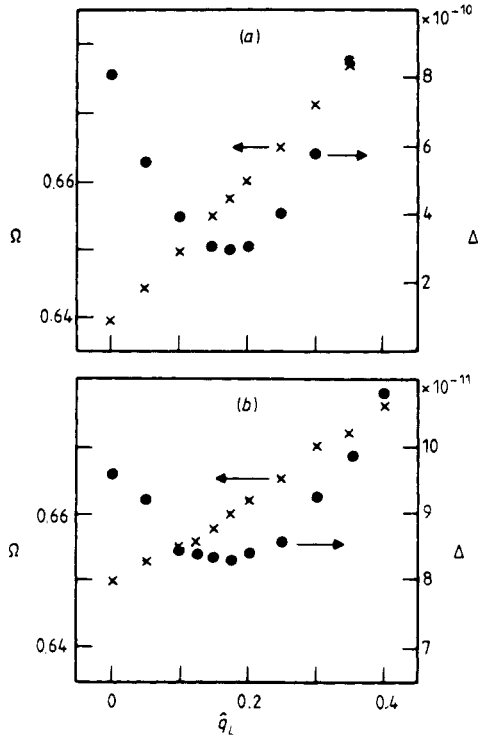

Figure 6. Variation of the effective correction exponent Ω (crosses, left scale) and of the mean square deviation (full circles, right scale) for fits with (*a*) two largest lattices $L = 95\,000$, $130\,000$ and (*b*) four largest lattices $L = 50\,000$, $95\,000$, $70\,000$, $130\,000$. The x-axis is in the parameter $\hat{q}_L$ of equation (12) ($\hat{q}_L = q_l/(\tau - 1 - 1/D)$).

† The plausibility arguments of Nienhuis (1982) for $y_2 = \sigma\nu\Omega = 2$ would mean $\Omega = 96/91$ for the corrections due to the irrelevant operator. This exponent is larger than all our estimates, suggesting that we see more important corrections, perhaps of the Aharony–Fisher type.

behaviour of

$$s^{\tau-1} \sum_{s' \geq s} n_{s'} = 0.0279 - 0.013\, s^{-0.66} + 0.175\, s^{1/D} L^{-1}, \tag{14}$$

in good agreement with the results of our previous fits of the partial sums.

7. Summary

In summary, we studied the corrections to scaling for percolation cluster numbers in two dimensions. We found at the percolation threshold the correction-to-scaling exponent $\Omega = 0.64 \pm 0.08$. Away from p_c, at $p = p_{max}$, the average effective $\Omega \cong 0.75$ is found to be slightly higher. We found that the ratio-like methods may overestimate the effective correction-to-scaling exponent Ω. The finite-size scaling analysis was made for our largest lattices. It seems likely that the leading corrections to scaling are not due to irrelevant scaling fields. It is possible that instead they arise from mixed terms in the scaling fields as postulated by Aharony and Fisher (1983).

Acknowledgments

We would like to thank E Brézin, Z Djordjevic, M E Fisher, E T Gawlinski, H J Herrmann, B Nickel, V Privman and M J Stephen for important discussions, the Boston University Academic Computing Center for machine time, and F Family, V Privman and C Unger for helpful comments on the manuscript.

Appendix 1. The Hoshen algorithm for large systems

A1.1. Random number generators

The Monte Carlo evaluation of the cluster numbers was done by the algorithm of Hoshen and Kopelman (1976), using a FORTRAN program on an IBM 3081 and 370/168 computers at Boston University and CDC Cyber 76 at Cologne University. To analyse one million sites on any of these computers required about 10 seconds; the single run for $70\,000 \times 70\,000$ thus took about 12 hours of time on the IBM 3081. A FORTRAN program has been published (Stauffer *et al* 1982) and therefore is not reproduced here.

For the very large lattices employed here special precautions are necessary. For $50\,000 \times 50\,000$ we used first the usual 'randu' random number generator (multiplication by 65 539 modulo 2^{31}). We then found reasonable results except that the correction-to-scaling exponent Ω appeared to be appreciably higher than for the $35\,000 \times 35\,000$ lattice and close to unity. Since this random number generator produces at most 2^{30} different random integers, and since the $50\,000 \times 50\,000$ lattice contains about twice as many sites, we then chose another method where one random number generator picks a random integer from a table produced by another random number generator (Ambegaokar *et al* 1973). The results were roughly the same except that the computer time was increased by about 50%. Finally we used the new random

number generator of Kirkpatrick and Stoll (1981) in a form which produces normalised real random numbers, supplied to us by C Mitescu (Pomona College). With this random number generator we could nearly reach the old computation speed again; and the resulting Ω (near 0.6) was compatible with what we found from the smaller lattice. We find this last generator the most trustworthy one and use only this result in our analysis of $50\,000 \times 50\,000$ lattice. The same random number generator was then used for $70\,000 \times 70\,000$. The $95\,000 \times 95\,000$ and $130\,000 \times 130\,000$ lattices were run on a CDC Cyber 76 computer, the latter simulation consuming 26 hours†. This is not only our largest system size but to our knowledge far exceeds the size of any other system simulated on computers (with the exception of a three million × three million lattice simulated by Dhar (1982) for directed percolation; that simulation may also be regarded as a curved one-dimensional walk of length three million). Our simulation thus may be the first large-scale test of the Kirkpatrick–Stoll random number generator. (Using Ising models and a different generator, Hoogland *et al* (1983) used ten times more random numbers and found subtle deviations from exact results.)

A1.2. Memory space and recycling

Another problem is memory space. The Hoshen algorithm in the form published by Stauffer *et al* (1982) requires for two dimensions that only one line of the lattice, and not the whole lattice, is stored at one time. The computer analyses the lattice as a typewriter writes on a page. But beside that array, called LEVEL by Stauffer *et al* (1982), one needs another array, called N there, which gives the label tree indicating which different labels belong to the same cluster. An integer, called INDEX, is increased by unity whenever a new cluster seems to start; then N(INDEX) is put equal to unity, and later may be changed into a different value. Thus the size of the array N needs to be at least as large as the total number of events where a new cluster seems to start.

How often is this the case? A new cluster seems to start whenever all previously analysed neighbours of a new site are empty, whereas the new site is occupied. For the triangular lattice, this happens with probability $p(1-p)^3$ since three of the six neighbours of the new site were analysed earlier. At $p = p_c = \frac{1}{2}$, this probability is $\frac{1}{16}$; thus more than six percent of the lattice sites seem to start a new cluster. It is of little help that most of these seemingly new clusters later turn out to be connected to an old cluster: the index has already increased by unity and requires therefore an additional memory space in the array N. Therefore, to use systems with more than one million sites, a 'recycling' of labels no longer used is necessary, as we will now describe in detail. Different forms of recycling have also been used in previous simulations of large lattices (Hoshen and Kopelman 1976, Eschbach *et al* 1981) but were not described there.

If we reached the end of, say, line 1000 in a $10\,000 \times 10\,000$ lattice we may separate all occupied sites into three classes: those which belong to clusters extending from the first or a later line to line 999 at most, which we call the finished clusters; those sites which belong to clusters having at least one site on line 1000, which we call the current clusters; and finally the future clusters, which start in line 1001 at the earliest and about which we know nothing yet. If we are interested in cluster numbers only, and

† Due to a programming error, the computer stopped working after 131 068 of the required 131 070 lines, and our analysis had to rely on the last intermediate output after 129 498 lines. Therefore, we denote this lattice as one of size $L = 130\,000$.

not in cluster–cluster correlation, we no longer need the labels $N(\text{INDEX})$ corresponding to the finished clusters; we only need to store the number and the size of the finished clusters. Thus we analyse once again line 1000 (i.e., we apply the subroutine or function 'class' to sites $i = 1, 2, 3, \ldots$ of line 1000) in order to know precisely what clusters we have up to now (Hoshen and Kopelman 1976; Stauffer *et al* 1982). By this process we check how the occupied sites are connected so far, and we treat each start of a new cluster on that line as the addition of another cluster, thus increasing further the index J, counting seemingly new clusters. If the classification subroutine results in a LABEL larger than the value of INDEX before recycling, then we know that this site is connected to a current cluster which had touched the line 1000 before; so we merely give this site a new label $\text{LEVEL}(i)$ equal to the value LABEL − INDEX (where INDEX stays as its value before recycling). If the occupied site i is a neighbour to another occupied site $i-1$ to the left, then it gets the same label: $\text{LEVEL}(i) = \text{LEVEL}(i-1)$. Finally, if the occupied site i has an empty left neighbour and the label resulting from the reclassification is not larger than the value of INDEX before the start of recycling, then a new current cluster seems to start here, and thus the current index J is increased by unity, the label tree N is adjusted accordingly, and $\text{LEVEL}(i)$ gets the value J-INDEX.

Having thus redefined the array LEVEL for this line, with proper labels starting from 1, we go through the labels of the finished clusters (between label = 1 and label = INDEX) and analyse the size distribution of the finished clusters. Finally, all elements $N(m)$ with labels m between 1 and INDEX can be forgotten since they belong to finished clusters; only labels between INDEX + 1 and the last value of J are important since they correspond to current clusters. Thus we shift the information contained in $N(\text{INDEX}+1), N(\text{INDEX}+2), \ldots, N(J)$ to the memory locations $N(1), N(2), \ldots, N(J - \text{INDEX})$. In this way, most of the array N becomes available for the future clusters.

For the $70\,000 \times 70\,000$ lattice, we used an array N of size 180 000 and started the recycling whenever the index came close to this maximum value, i.e., whenever it was larger than about 157 000. In total, we need a memory of about one megabyte. Recycling occurred about every 30 lines; after a recycling the value of INDEX had shrunk to about 10 000. Thus for the long runs ($50\,000 \times 50\,000$, $70\,000 \times 70\,000$, $95\,000 \times 95\,000$, and $130\,000 \times 130\,000$) we also stored intermediate results on the disc to allow the whole job to run in several installments. The end of recycling is an appropriate time to put the status of the lattice on a disc without wasting too much memory space. Basically our method, due to one of us (HN), has the advantage over that of Hoshen and Kopelman (1976 and Hoshen, private communication) that it stores only one line, whereas Hoshen and Kopelman (1976) always store two lines. Thus it frees the amount of memory used for storing the extra line and makes it available for increasing the size of the array N; this in turn reduces the number of recycling and consequently execution time. The advantage is greater when recycling is frequent.

While the simulation of even larger lattices would not be impossible in terms of computer time and memory, another problem would appear for lattices of size greater than $100\,000 \times 100\,000$. The size of the largest cluster at the critical point would be larger than $(2^{31} - 1)$, making that size negative on IBM computers. Negative sizes, on the other hand, are used to connect different labels, and could lead to catastrophic results; far above p_c it would occur already for $50\,000 \times 50\,000$ and $70\,000 \times 70\,000$ lattices. We avoided this problem simply by using a CDC computer for larger size lattices since CDC machines have 60 bit words, much larger than IBM.

Appendix 2. Potts model argument

In this appendix, we argue that the underlying symmetry of the q-state Potts model suggests the absence of linear mixing in the temperature-like scaling field g_t as well as in the field-like scaling field g_h. Since percolation is considered to be a $q \to 1$ limit of the q-state Potts model, this argument appears to favour the absence of such mixing for percolation also. In what follows, we shall adopt the q-state Potts model language for general integral q. Thus, we consider the Hamiltonian

$$\mathcal{H} = -\sum_{(i,j)} J\boldsymbol{s}_i \cdot \boldsymbol{s}_j - \sum_i \boldsymbol{H} \cdot \boldsymbol{s}_i, \tag{A2.1}$$

where the variables $\boldsymbol{s}_i$ at each lattice site i assume the vector values $\boldsymbol{e}^\alpha$ for some α $(=1, 2, \ldots, q)$ each of which is pointing toward one of the vertices of a $(q-1)$-dimensional multihedron, and $\boldsymbol{H}$ is an external field favouring one of these vectors.

Let us assume an exact, asymptotic scaling form for the singular part G_s of the free energy:

$$G_s \simeq |g_t|^{2-\alpha} Y(g_h/|g_t|^\Delta), \qquad \Delta = \beta\delta = 1/\sigma, \tag{A2.2}$$

where g_t and g_h are in general nonlinear scaling fields (coefficients omitted),

$$g_t = t(1 + t + h + \ldots) + h + \ldots, \tag{A2.3}$$

$$g_h = h(1 + t + h + \ldots) + t + \ldots, \tag{A2.4}$$

with $t = (T - T_c)/T_c$ and $h = (\boldsymbol{H}/k_B T)\boldsymbol{e}^1 = \boldsymbol{h} \cdot \boldsymbol{e}^1$. We argue that g_t cannot have a linear term in h and that g_h cannot have a linear term in t. (In fact, the latter claim can almost be *shown* based on a different argument; see below.)

The scaling field g_t is an analytic function of t and $\boldsymbol{h}$, and so is g_h. Now, g_t must be invariant under a symmetry operation on the system because it couples to $|\boldsymbol{s}|^2$ at criticality, and g_h should transform like a projection of $\boldsymbol{s}$ under the same operation. In our case, the permutation group of the q possible states (or directions of order) is the symmetry operation in the absence of $\boldsymbol{h}$; however, in the presence of $\boldsymbol{h}$, this field must also be rotated to leave the Hamiltonian invariant. For example, for $q = 3$, when the order $\boldsymbol{s}$ is rotated from $\boldsymbol{e}^1$ to $\boldsymbol{e}^2$, one must also change $\boldsymbol{h} = h_0\boldsymbol{e}^1$ to $h_0\boldsymbol{e}^2$. Thus, the only allowed occurrence of $\boldsymbol{h}$ in g_t should be invariant combinations under these transformations. Similarly, since $\boldsymbol{h}$ itself transforms like $\boldsymbol{s}$, g_h must be a linear term in $\boldsymbol{h}$ multiplied by terms invariant under the transformation. The allowed combinations of $\boldsymbol{h}$ in g_t and in g_h/h are thus, e.g.,

$$\boldsymbol{h} \cdot \boldsymbol{h} = h_0^2, \qquad \text{or} \quad \sum_{\substack{\alpha \\ l,m,n}} e_1^\alpha e_m^\alpha e_n^\alpha h_l h_m h_n, \tag{A2.5}$$

or higher orders. Incidentally, the latter vanishes for $q = 2$ (Ising), leaving even fewer invariants than for $q \neq 2$. Thus, it is possible to have fewer invariants for special values of q, but not more. A linear term such as $\boldsymbol{h} \cdot \hat{\boldsymbol{n}}$ (where $\hat{\boldsymbol{n}}$ is a fixed vector) is clearly not permissible for any q.

If we further assume that nothing strange happens as $q \to 1$, then no linear mixing is allowed for percolation, either. Actually, the argument is much more general: if any symmetry operation (locally about the critical point) transforms $\boldsymbol{h}$ at all, then no linear term in h can be present in g_t, for any Potts model.

Moreover, the claim that g_h has no linear term in t can be placed on even more secure footing. This observation follows quite simply by considering the scaling law (A2.2) (which we assume) and the additional assumption that all singularities expressed in (A2.2) occur at $h=0$ with some actually occurring at $t<0$. (We consider the $g_t<0$ branch of $Y(x)$.) The singularities at $h=0$, $t<0$ must be those of $Y(x)$ since the prefactor $|g_t|^{2-\alpha}$ is not singular there. If $Y(x)$ is singular at, say $x=x_0$, then all points (t, h) satisfying $g_h/|g_t|^{\Delta}=x_0$ are also singular. We would then in general have an equation mixing t and h for a trajectory of singularities. The only sensible way to avoid singularities for $h\neq 0$ is by identifying $x_0=0$ (and $g_h=0$ if $h=0$).

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