J. Phys. A: Math. Gen., Vol. 12, No. 8, 1979. Printed in Great Britain

Monte Carlo experiments on cluster size distribution in percolation

J Hoshen†‖, D Stauffer‡, George H Bishop§, Ralph J Harrison§ and George D Quinn§

† Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA
‡ Institut für Theoretische Physik, Universität, Zülpicherstr. 77, 5000 Köln 41, West Germany
§ Army Materials and Mechanics Research Center, Watertown, Massachusetts 02172, USA

Received 6 October 1978

Abstract. Cluster statistics in two- and three-dimensional site percolation problems are derived here by Monte Carlo methods. The average number n_s of percolation clusters with s occupied sites each is calculated by up to 19 runs on a 4000×4000 triangular lattice near p_c. Our data support the two-exponent scaling assumption $n_s \propto s^{-\tau} f(z')$, where $z' = (p/p_c - 1)s^{\sigma}$. At the percolation threshold $p = p_c$ we find for s up to 10^6 a rough agreement with the expected power law $n_s \propto s^{-\tau}$ over 12 decades in n_s; we can approximate the leading correction term near $s \sim 10^2$ by $n_s \propto s^{-\tau}(1 - 1{\cdot}2\, s^{-2/3})$. If the ratio $v_s = n_s(p)/n_s(p_c)$ is plotted against z', then all data follow the same curve $v_s = f(z')$ for different p. This scaling function $f(z')$ has a finite slope at $z' = 0$, has a maximum $f(z'_{max} \simeq -0{\cdot}8) \simeq 5$ for p below p_c, and decays rapidly for $z' \to \pm\infty$. For $s \to \infty$ at fixed p this rapid decay corresponds to $\ln n_s \propto -s^{1/2}$ above p_c and $\ln n_s \propto -s$ below p_c. Apart from finite-size corrections we find the second moment $\chi \equiv \Sigma s^2 n_s$ diverges as $|p - p_c|^{-\gamma}$, with $\gamma \simeq 2{\cdot}4$, on both sides of the phase transition; the amplitude ratio $\chi(p < p_c)/\chi(p > p_c)$ is about 200. The fraction of occupied sites belonging to the infinite cluster vanishes as $(p - p_c)^{\beta}$, with $\beta \simeq 0{\cdot}13$. In three dimensions using system sizes up to $400 \times 400 \times 400$ the two-exponent scaling function is also supported, with the same universal function $f(z')$ valid for both the simple cubic and BCC lattices. $f(z')$ has a maximum $f(z'_{max} \simeq -0.8) \simeq 1{\cdot}6$. The amplitude ratio is approximately 11. Our conclusions are in general consistent with but more complete than other recent Monte Carlo work by Stoll and Domb, Leath and Reich, and Nakanishi and Stanley.

1. Introduction

Recent Monte Carlo work by Stoll and Domb (1978), Leath and Reich (1978) and Nakanishi and Stanley (1978) on the cluster size distribution in two-dimensional percolation clarified many questions previously unsolved or controversial. Nevertheless, none of these studies investigated the whole range of problems, since Stoll and Domb looked at cluster numbers above the percolation threshold p_c, Leath and Reich at $p \leqslant p_c$ only, and Nakanishi and Stanley gave results not for the cluster numbers directly but for a related equation of state. Also, these studies were restricted to two dimensions. The present paper tries to fill this gap by a unified analysis of Monte Carlo

‖ Partially supported by Army Research Office Grant DAAG 29-78-G-0073 and National Institutes of Health Grant 2 R01 NS08116-10A1.

numbers above, at and below p_c in two and three dimensions. We understand that the work of Nakanishi and Stanley will be continued in the same direction as investigated here; thus by comparing these papers the reader will get a good impression about the open and the solved problems for percolation cluster numbers.

In the (site) percolation problem (Essam 1972, Kirkpatrick 1973) the points of a periodic lattice are randomly and independently occupied with the probability p. A cluster is a group of occupied sites connected by nearest-neighbour distances (except for the BCC lattice where our data refer to sites connected by both nearest- and next-nearest-neighbour distances—the BCC–1,2 site problem). Our Monte Carlo studies were made by techniques described elsewhere (Quinn *et al* 1976b, Hoshen and Kopelman 1976). In these studies pseudo-random numbers distributed uniformly in the interval (0, 1), generated by a congruence method, are assigned to each lattice site. An arbitrary random number is chosen to start the sequence; a second use of the same 'starter' will produce the identical sequence of pseudo-random numbers. The sites are designated as occupied or unoccupied, depending on whether the random number assigned to that site is less than or greater than p. Our Monte Carlo studies were made with up to 19 independent random number starters per concentration in a 4000×4000 triangular lattice ($p_c=\frac{1}{2}$), and also with a simple cubic lattice of size $400\times400\times400$ ($p_c\sim0{\cdot}31$) using a single random starter at four concentrations. We also used 4–8 random number starters and a $\pm10\%$ range of concentrations in a $100\times100\times100$ simple cubic lattice, 1–15 random number starters per concentration in a simple cubic lattice with $86\times86\times86$ sites, and 3–16 starters in a BCC lattice of $2(40)^3$ or 128 000 sites. Some analyses of the results in the last two lattices have been given in Quinn *et al* (1976a, b) and in Harrison *et al* (1978). The two large systems are, to our knowledge, the largest systems thus far investigated by Monte Carlo methods in two or three dimensions. In general our statistics are about as good or better than those of previous work. Current reviews of percolation problems are being prepared by Essam, by Pfeuty and Guyon, and by Stauffer (private communications).

We are interested here in the average number $n_s=n_s(p)$ of clusters (per lattice site) containing s occupied sites each. In analogy with other critical phenomena, a two-exponent scaling assumption (Stauffer 1975)

$$n_s(p)\propto s^{-\tau}f(z), \qquad z\equiv(p-p_c)s^{\sigma}, \tag{1}$$

for $s\to\infty$, $p\to p_c$ is tested in the present work, as was done also by Leath and Reich (1978). The usual critical exponents of percolation theory are then related to equation (1) by $2-\alpha=(\tau-1)/\sigma$, $\beta=(\tau-2)/\sigma$, $\gamma=(3-\tau)/\sigma$, $\delta=1/(\tau-2)$, or $\sigma=1/\beta\delta=1/(\beta+\gamma)$ and $\tau=2+1/\delta$. A block-spin renormalisation group argument in favour of equation (1) was recently given by Kunz and Payandeh (1978) (see also Stephen 1977). The scaling assumption of Essam and Gwilym (1971) for the equation of state, which was confirmed by Nakanishi and Stanley, is a necessary but not sufficient condition for the validity of equation (1). Leath (1976) originally proposed a 'Gaussian' *ansatz* with three free exponents τ, ψ, ϕ; but Leath and Reich (1978) found from more accurate data that two of them are equal: $\psi=\phi=\sigma$. Domb (1974) suggested a form with one free exponent τ; this suggestion was not confirmed by later results (Domb 1976, Sykes *et al* 1976, Amit 1976, Priest and Lubensky 1976). Our paper will collect further evidence for the equality of Leath's ψ and ϕ. Thus equation (1) seems to be the only scaling assumption available which still seems plausible. Of course that fact does not prove this assumption to be correct.

In the numerical investigation of cluster numbers near the percolation threshold it is often convenient to normalise them as

$$v_s(p) = n_s(p)/n_s(p_c). \tag{2a}$$

For these ratios the scaling equation (1), with $f(0)$ normalised to unity, takes the simple form

$$v_s(p) = f(z). \tag{2b}$$

The ratios v_s are useful if we look at the regime $p > p_c$, where $n_s(p)$ is smaller than $n_s(p_c)$, or if we have more data at $p = p_c$ than at $p \neq p_c$ (as is the case in our present studies); the v_s are less practical if $n_s(p)$ is known more accurately than $n_s(p_c)$, as is often the case in the work of Leath and Reich (1978).

If an exponent ζ is defined (Bakri and Stauffer 1976) by

$$\ln n_s \propto -s^{\zeta}, \qquad s \to \infty, \tag{3a}$$

a definition not restricted to the region of p close to p_c, then Kunz and Souillard (1978) have shown, in agreement with earlier numerical studies (Stauffer 1976, Flammang 1977), that $\zeta = 1$ for sufficiently small p, and $\zeta = 1 - 1/d$ in d dimensions for sufficiently large p. Thus we now try to find out, as has been done already by Stoll and Domb ($\zeta = \frac{1}{2}$ above p_c) and Leath and Reich ($\zeta = 1$ below p_c), if these predictions can be extrapolated to the critical region, i.e. if

$$\zeta(p > p_c) = 1 - 1/d, \qquad \zeta(p < p_c) = 1, \tag{3b}$$

for all $p \neq p_c$. In that case the scaling function $f(z)$ for large $|z|$ varies asymptotically as $\ln f(z) \propto -|z|^{-\zeta/\sigma}$ if the convergence of the $n_s(p)$ to their scaling form (1) is sufficiently uniform.

Our two-dimensional results at, above and below p_c are analysed in §§ 2–5, §6 gives a short account of our three-dimensional work, and our conclusions are summarised in § 7.

2. Cluster numbers at p_c in two dimensions

To analyse our cluster numbers n_s we combine them into groups in order to simplify the analysis and to reduce statistical fluctuations. Following Quinn *et al* (1976a, b) we chose as groups the size intervals from $s = 2^i$ to $s = 2^{i+1} - 1$, $i = 0, 1, 2, \ldots$. For each group we took as the average s the geometric mean (Stauffer 1975) of the upper and lower end of the size interval, an approximation which should be the better the closer n_s is approximated by an s^{-2} decay law. As critical exponents in two dimensions we take the results of Sykes *et al* (1976): $\beta = 0{\cdot}138$, $\gamma = 2{\cdot}43$ and thus $\sigma = 0{\cdot}39$ and $\tau = 2{\cdot}05$. In § 5 we will show that these values for β and γ are consistent with direct determination from our Monte Carlo data. (Domb and Pearce (1976) found $\alpha = -0{\cdot}668 \pm 0{\cdot}004$ in the triangular lattice, which gives $\gamma \simeq 2{\cdot}39$ from $2 - \alpha = \gamma + 2\beta$, in even better agreement with our later Monte Carlo result $\gamma = 2{\cdot}36 \pm 0{\cdot}1$. However, Reynolds *et al* (1978) give $\gamma = 2{\cdot}435 \pm 0{\cdot}035$; and if Klein *et al* (1978b) are correct in stating that $\nu = \ln\sqrt{3}/\ln\frac{3}{2}$ exactly, then $d\nu = 2 - \alpha$ gives $\alpha = -0{\cdot}71$ and again $\gamma \simeq 2{\cdot}43$.)

Figure 1 shows the number n_s of clusters per lattice site at $p = p_c = \frac{1}{2}$, based on 19 runs and 16 000 000 sites. On this scale the cluster numbers n_s vary over 12 decades

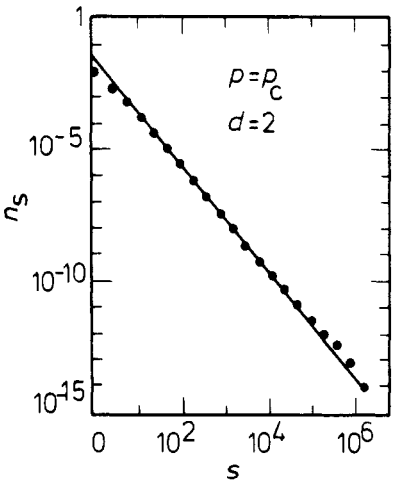

Figure 1. Variation of n_s, the average number (per lattice site) of clusters with s occupied sites each, with size s at the percolation threshold $p = p_c = \frac{1}{2}$. The full line is the prediction of Gaunt and Sykes (1976), based on an extrapolation from small cluster sizes below $s = 15$.

and follow, for cluster sizes up to 10^6, a simple power law indicated by a straight line in the log–log plot, just as required by equation (1) at $z = 0$:

$$n_s(p_c) = q_0 s^{-\tau}. \tag{4}$$

The line through the data is not a fit but the prediction from series expansions (Gaunt and Sykes 1976) with $q_0 = 0{\cdot}03$; the general agreement is excellent.

Closer inspection, however, shows significant deviations from the simple power law (equation (4)) at both ends of the figure. For s below 10 both the Monte Carlo data as well as the exact expressions (Sykes and Glen 1976; see also the table of Flammang 1977) are appreciably smaller than those predicted by equation (4). Similar deviations were also observed for Ising model clusters (Stoll *et al* 1972, Binder and Müller-Krumbhaar 1974) and in earlier percolation studies (Stauffer 1975, Quinn *et al* 1976a, b). For example, theoretically the normalised number n_1 of isolated occupied sites should be $p(1-p)^6 = \frac{1}{128}$ at $p = \frac{1}{2}$ in the triangular lattice, whereas equation (4) with $q_0 = 0{\cdot}03$ predicts $n_1 = 0{\cdot}03$, or four times larger than the exact value. The Monte Carlo data obtained in 19 runs on a 4000×4000 lattice at $p = \frac{1}{2}$ show agreement to within 0.3% of the exact results; that is, theoretically 2375 000 such $s = 1$ clusters should be expected, while experimentally we found 2382 505 such clusters. This illustrates that scaling laws like equation (4) are only valid for large clusters, although when one considers ratios $v_s = n_s(p)/n_s(p_c)$ some of these deviations for small clusters may cancel out.

For s near 10^5 also some deviations can be seen in figure 1; these deviations can be seen more clearly if the same data are replotted as $s^{\tau} n_s$ against ln s. Actually, to reduce the statistical error, figure 2 gives the partial sums

$$s^{\tau-1} \sum_{s' \geqslant s}^{\infty} n_{s'}$$

for $s = 2^i$, $i = 0, 1, 2, \ldots$. If equation (4) were exact, then these partial sums would all

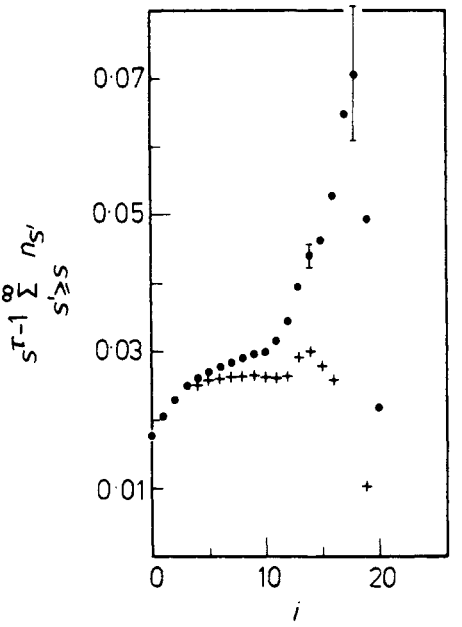

Figure 2. Variation with $\log s$ of the partial sums $s^{\tau-1}\sum_{s'\geqslant s}^{\infty} n_{s'}$ for $s = 2^i$ at $p = p_c$ (full circles). The crosses give data at $p = p_c + 0{\cdot}001$, i.e. at the shifted p_c^s of § 5.

be equal to the same constant $q_0/(\tau-1)$ if the sums were replaced by integrals. In figure 2 the scales are much finer than in figure 1, and we now see drastic deviations from the scaling law (4). Two regions can be distinguished; for small clusters the data points are somewhat lower than the expected value near 0·03; and for s above 10^3 they are appreciably higher (except for the last point near $s = 10^6$). The first effect was explained above: we are not yet in the asymptotic scaling region of large s. (The error from the replacement of sums by integrals is in the opposite direction.) The second effect is interpreted as showing the influence of the system boundaries on the large clusters (see also §§ 5 and 6). Free boundaries were used in modelling the triangular lattice; cluster sizes larger than 16 000 000 cannot therefore occur, and very large clusters ($s \geqslant 10^6$) are broken up by the boundaries into many smaller ones. Thus a cluster deficiency in the largest available cluster size group is compensated by a cluster excess for smaller sizes, just as figure 2 shows. This hypothesis is supported by a comparison of a 4000×4000 run with a 2000×2000 run by Hoshen and Kopelman (1976), where around $s = 10^4$ the smaller system had larger (normalised) cluster numbers n_s than the larger system. Even for $s = 1$ we regard the deviation by 0·3% mentioned above as statistically significant and as due to finite-size effects. Also for larger s up to 14, where exact results exist (Sykes and Glen 1976), the relative deviation between experiment and theory increases slightly with increasing cluster size. (In Leath's (1976) method no such size effects occur, but it requires an arbitrary cut-off in s which was taken near 10^3, the same cluster size where our data also become inaccurate.)

To describe the deviations at small s from the asymptotic behaviour for large s one may in general postulate

$$n_s \propto s^{-\tau} f(z) - s^{-\tau-x} f_1(z) + \ldots, \tag{5a}$$

with a correction-to-scaling exponent x to be fitted on experiment. Right at p_c this assumption leads to

$$n_s = q_0 s^{-\tau}(1 - Xs^{-x} + \ldots). \tag{5b}$$

In this case also the partial sums plotted in figure 2 would carry such a correction factor $(1 - \text{constant} \times s^{-x})$. Figure 3 gives a rough impression that x is larger than 0·224

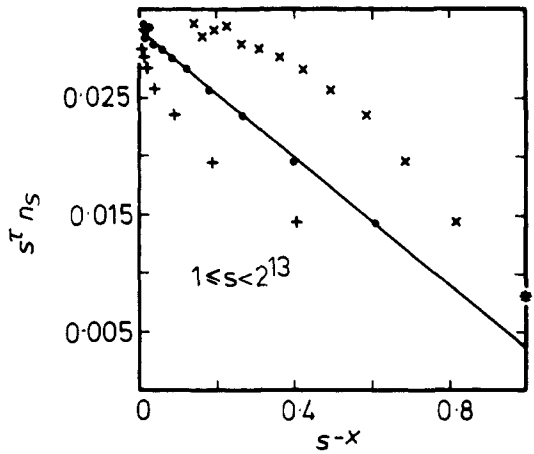

Figure 3. Variation with s^{-x} of the same partial sums as in figure 2, at $p = p_c$, with $x = 0{\cdot}224$ (×), 0·55 (●) and 1 (+). If $s^{\tau} n_s$ varied as 1-constant × s^{-x}, these data would follow a straight line.

$(=2\psi - 2\phi$ in Leath's original suggestion (Leath 1976)) and smaller than unity, the value taken by Quinn *et al* (1976a, b). With $x \geqslant \frac{1}{2}$ we get a reasonable straight line in figure 3, corresponding to a fit on equation (5*b*). A more accurate fit, based on the n_s themselves and including the exact n_s for small s, leads to

$$q = 0{\cdot}0304, \qquad X = 1{\cdot}19, \qquad x = 0{\cdot}67 \pm 0{\cdot}1, \tag{6}$$

in reasonable agreement with the exponent $x = 0{\cdot}75 \pm 0{\cdot}05$ from Gaunt and Sykes (1976) and consistent with the renormalisation group result that the correction exponent is of order unity (Houghton *et al* 1978; G Grest, private communication). (If we were to neglect the correction term, treat τ as a free exponent and fit it on n_s between $s = 10^2$ and $s = 10^4$, we would get $\tau \simeq 2{\cdot}02$, which is somewhat too low (Gaunt and Sykes 1976).)

We also calculated in our 19 runs the cluster numbers at several concentrations slightly away from p_c, with $|p - p_c| \sim 10^{-3}$. Figure 4 shows the resulting ratios $v_s = n_s(p)/n_s(\frac{1}{2})$ against the scaling variable $z = (p - p_c)s^{\sigma}$. Equation (2*b*) requires that these ratios all fall on the same curve for different $p - p_c$, and indeed they do. Thus we can confirm already very close to p_c the conclusions of Leath and Reich below p_c, and of Nakanishi and Stanley for the equation of state, that two-exponent scaling seems to work. Moreover, in this region the scaling curve $f(z)$ or $\ln f(z)$ is linear in its variable z, with

$$(\mathrm{d} \ln f/\mathrm{d}z)_{z=0} = (\mathrm{d}f/\mathrm{d}z)_{z=0} \simeq -7{\cdot}1. \tag{7a}$$

From the exact n_s for small s we extrapolate this derivative to be about $-7{\cdot}3$. Thus the

truth might be $-7{\cdot}2 \pm 0{\cdot}1$. Both the exact results and the Monte Carlo estimates are shown in figure 5. We could not determine reliably the second derivative from our Monte Carlo data; from the exact result for $s \leqslant 14$ we extrapolate in figure 5 to obtain

$$(\mathrm{d}^2 \ln f/\mathrm{d}z^2)_{z=0} = -15 \pm 1. \tag{7b}$$

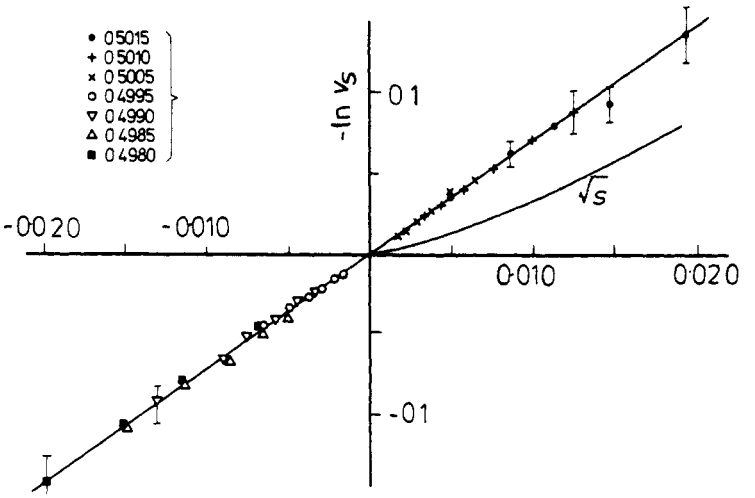

Figure 4. Test of scaling, equation (1), very close to p_c. Scaling requires curves with different symbols, corresponding to different p, to coincide. $v_s = n_s(p)/n_s(p_c)$. The curve with label $\sqrt{s}$ is an extrapolation from larger values of $z = (p - p_c)s^{\sigma}$.

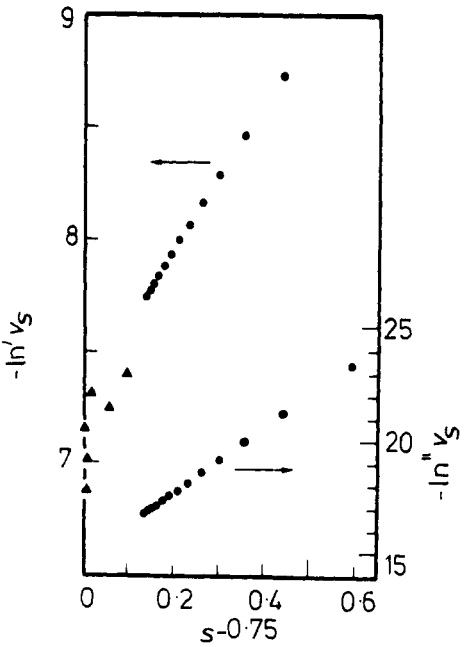

Figure 5. Determination of the derivatives $\ln' v_s = \mathrm{d}(\ln v_s)/\mathrm{d}z$ and $\ln'' v_s = \mathrm{d}^2(\ln v_s)/\mathrm{d}z^2$. Full triangles refer to our Monte Carlo data, full circles to exact results from Sykes and Glen (1976).

From these derivatives one can calculate (Leath and Reich 1978) the fluctuations in the perimeter t_s of s clusters, and we find, at $p = p_c = \frac{1}{2}$,

$$\langle t_s^2 \rangle - \langle t_s \rangle^2 = 2s - 3{\cdot}7s^{2\sigma} + 3{\cdot}6s^{\sigma}. \tag{7c}$$

For s above 20 this prediction agrees well with the Monte Carlo results for the width of the perimeter distribution (Leath and Reich 1978, figure 13). Since the second term on the RHS of equation (7c) is nearly equal to the first term, one would have to go to extremely large clusters to make the term $2s$ clearly dominating. This fact explains why from the exact results for small s (Stauffer 1976, Flammang 1977) a wrong variation of this width with s was predicted.

In Leath's (1976) original proposal the derivative $\mathrm{d}(\ln v_s)/\mathrm{d}p$ varies at $p = p_c$ with $s^{2\phi-\psi} = s^{0{\cdot}29}$, whereas in the two-exponent *ansatz* of equation (1) it varies as $s^{\sigma} = s^{0{\cdot}39}$. Our figure 6 shows that this derivative in our Monte Carlo study varies roughly as $s^{0{\cdot}38}$, consistent with equation (1). Thus we can confirm the conclusion of Leath and Reich (1978) that $\phi = \psi$ and that only two exponents are needed to describe the scaling region.

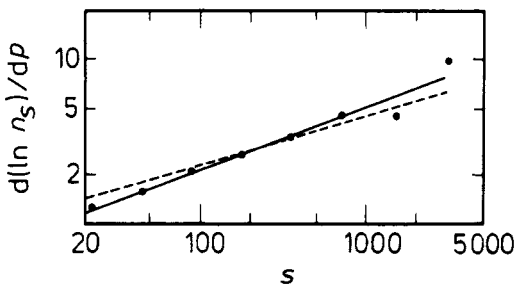

Figure 6. Log–log plot of $\mathrm{d}(\ln n_s)/\mathrm{d}p$ (in arbitrary units) against s at $p = p_c$. The full-line fit has the slope 0·38. Two-exponent scaling predicts a slope of 0·39, three-exponent scaling (Leath 1976) a slope of about 0·29 (broken line).

3. Cluster numbers above p_c

Figure 7 again is a scaling plot of the ratios $v_s = n_s(p)/n_s(p_c)$ against the scaling variable $z = (p - p_c)s^{\sigma}$, based on three runs in our 4000×4000 lattice. Only clusters with sizes between 16 and 10^3 were plotted to avoid the errors due to small clusters or small lattices shown in figure 2. Again different symbols in figure 7, corresponding to different p, follow the same curve within about 10% or better, in agreement with the scaling assumption ((1) and (2b)). The full curve is the extrapolation of Wolff and Stauffer (1978), which was based on the exact cluster numbers of Sykes and Glen (1976) for s below 15; it agrees surprisingly well with the Monte Carlo data, except for errors of about 10% near $z = 0{\cdot}2$. (Also below p_c similar agreement between that extrapolation and our Monte Carlo data was found.) The straight line in figure 7 is the tangent through the origin as determined from the more accurate data of equation (7a) and figure 4. We now see clearly, in agreement with Stoll and Domb (1978) but in contrast to the Fisher droplet model (Fisher 1967) and earlier studies (Stauffer 1975) based on less accurate data, that there is some curvature in the semilogarithmic plot of figure 7; that means the cluster numbers do not simply follow $\ln v_s \propto -z$, i.e. $n_s \propto s^{-\tau} \mathrm{e}^{-\epsilon s^{\sigma}}$ with $\epsilon \propto p - p_c$. This simple 'Fisher model' formula can now be excluded on the basis of these

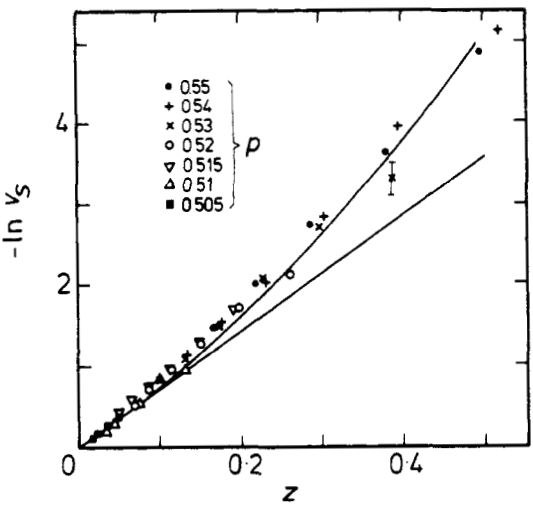

Figure 7. Test of scaling above p_c, as in figure 4. The straight line is the tangent to the origin from figure 4, the full curve the extrapolation of Wolff and Stauffer (1978).

Monte Carlo data and should be replaced by the more general scaling assumption (1), which of course was developed on the basis of the Fisher model.

If we assume that our data are already in the asymptotic region to determine the exponent ζ of equation (3), then the upward curvature in figure 7 suggests $\zeta > \sigma$. In figure 8 we plot for $p = 0{\cdot}55$ the same data again, in three different ways: as a function of $z \propto s^{\sigma}$, as a function of $z^{1/\sigma} \propto s$, and as a function of $z^{1/2\sigma} \propto s^{1/2}$, corresponding to the exponents $\zeta = \sigma$, $\zeta = 1$, and $\zeta = \frac{1}{2}$, respectively. Clearly the data with $\zeta = \frac{1}{2}$ give the best straight line in this semilogarithmic plot, and the same is true if we look at all data in figure 7 (not shown). Thus above p_c even intermediate cluster sizes below 10^3 sites, with

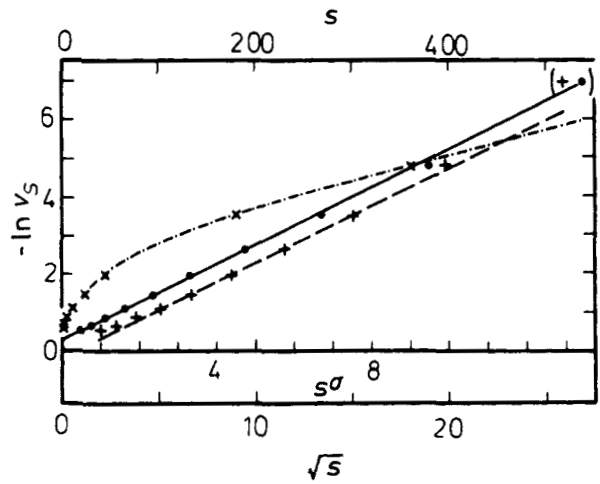

Figure 8. Test of asymptotic decay of cluster numbers above p_c at $p = 0{\cdot}55$. The ratios $v_s = n_s(p)/n_s(p_c)$ are plotted logarithmically against s (×, chain curve), against $s^{1/2}$ (●, full line) and against $s^{\sigma} = s^{0{\cdot}39}$ (+, broken line). The full line gives the best fit, suggesting $\zeta = \frac{1}{2}$ already in this size range.

$z \sim 0{\cdot}1$, seem to be sufficiently large to allow the attainment of the asymptotic exponent

$$\zeta(p > p_c) = \tfrac{1}{2}, \tag{8}$$

in full agreement with the Kunz–Souillard theorem, equation (3*b*) (see also Hankey (1978) for related theories), and also with Monte Carlo work of Stoll and Domb (1978) who found $\zeta = 0{\cdot}48$ to $0{\cdot}49$ in the square lattice, using better statistics but smaller lattices than we used.

For very small z we see deviations from the simple $\ln v_s \propto \sqrt{s}$ behaviour suggested by figure 8. If we take a straight line through the origin fitting in figure 8 the data at intermediate z as a function of $s^{1/2}$, then this straight line $\ln v_s \propto s^{1/2}$ corresponds to the curve labelled $\sqrt{s}$ in figure 4. It deviates on the fine scale of that figure significantly from the Monte Carlo data very close to p_c. This deviation has to be expected, however, since the function $v_s = f(z)$ is likely to be analytic in z and therefore cannot vary as $\ln f \propto z^{1/2\sigma}$ for $z \to 0$, even if it varies with this power for all intermediate and large z. However, in terms of the function f or the cluster numbers n_s, the deviations from the simple decay law $\ln v_s \propto -s^{1/2}$ are relatively small compared, for example, with the strong variation of $n_s(p_c)$ with s at the critical point. Thus $n_s \propto s^{-\tau} \exp(-\text{constant} \times s^{1/2})$, albeit not exact, is a reasonable order-of-magnitude approximation; the implications of that conclusion, together with further data confirming it, are discussed by Bauchspiess and Stauffer (1978) in connection with nucleation theory.

4. Cluster numbers below p_c

The behaviour of the cluster numbers n_s below the percolation threshold is more complicated than above p_c, and we made only one run in the 4000×4000 lattice. It has been known for some time that $n_s(p)$ as a function of p has a maximum at $p_{max} = p_{max}(s)$ below p_c. This maximum is easily seen: for example, we have $n_1 = p(1-p)^6$ for $s = 1$ (single occupied sites) in the triangular lattice, which has a maximum at $p_{max} = \frac{1}{7}$, far below $p_c = \frac{1}{2}$; and $n_1(p_{max})/n_1(p_c)$ is about 7. The insert in figure 9 shows as an example the variation of n_s with p for $1024 \leq s \leq 2047$. This maximum makes an analysis of the

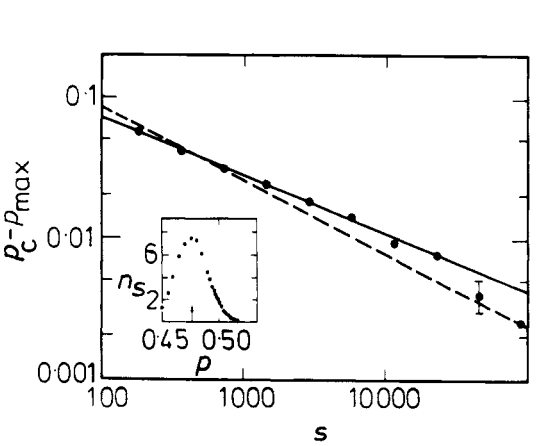

Figure 9. Log–log plot of $p_{max} - p_c$ against cluster size s. Our fit by the full line has the slope $-0{\cdot}40$; the broken line has the slope -0.51. The insert shows as an example the variation of n_s with p near $s = 10^3$.

asymptotic decay in the sense of equation (3) much more difficult below p_c than above p_c.

From our cluster numbers (more precisely, from sn_s) we determined the position $p_{max}(s)$ of the maximum in $n_s(p)$. Figure 9 shows $p_c - p_{max}$ as a function of cluster size. Except for the last two points near $s = 10^5$ the data fit surprisingly well a straight line in this log–log plot,

$$p_c - p_{max} = (0.44 \pm 0.03) s^{-0.40 \pm 0.02}, \tag{9a}$$

a result much more accurate than the earlier analysis $p_c - p_{max} = 0{\cdot}38 s^{-0.36}$ of Stauffer (1975). The two-exponent scaling assumption ((1) and (2*b*)) predicts this maximum to occur at some constant value of $z = (p - p_c)s^{\sigma}$, i.e. $p_c - p_{max} \propto s^{-0.39}$. On the other hand, the three-exponent *ansatz* (Leath 1976) gives $p_c - p_{max} \propto s^{-\psi} = s^{-0.51}$. Again, in agreement with Leath and Reich (1978), we find the two exponent *ansatz* to be better than the three-exponent assumption which would correspond to the broken line in figure 9. Thus the scaling function $f = f(z)$ of equation (1) has a maximum at

$$z_{max} = (p_{max} - p_c)s^{\sigma} = -0{\cdot}41 \pm 0{\cdot}03. \tag{9b}$$

Wolff and Stauffer (1978) predicted z_{max} to be near $-0{\cdot}45$ in the triangular lattice, in satisfactory agreement with the more acurate Monte Carlo data.

Figure 10 shows the ratios v_s against the scaling variable z for $p_{max} \leqslant p \leqslant p_c$. Data for different p follow the same curve, confirming again the scaling assumption (2*b*); for simplicity, figure 10 uses the same symbols for different p. The tangent to the origin is taken again from equation (7*a*). At the maximum $z = z_{max}$ we find a value $f_{max} = f(z_{max}) = n_s(p_{max})/n_s(p_c)$ of

$$f_{max} = 4{\cdot}9 \pm 0{\cdot}1. \tag{10}$$

This result is somewhat higher and more reliable than the extrapolation $f_{max} = 4{\cdot}5 \pm 0{\cdot}2$ of Stauffer (1976); 'universality' assumptions require f_{max} to be the same for all normal two-dimensional lattices (Marro 1976).

The decay of cluster numbers beyond this maximum for p below p_{max} is shown in figure 11, again confirming the scaling assumption (2*b*). The straight line through these

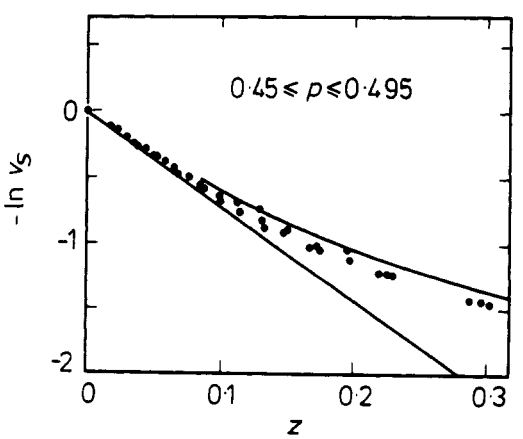

Figure 10. Test of scaling below p_c, as in figures 4 and 7. The tangent comes from figure 4, the full curve from the extrapolation of Wolff and Stauffer (1978).

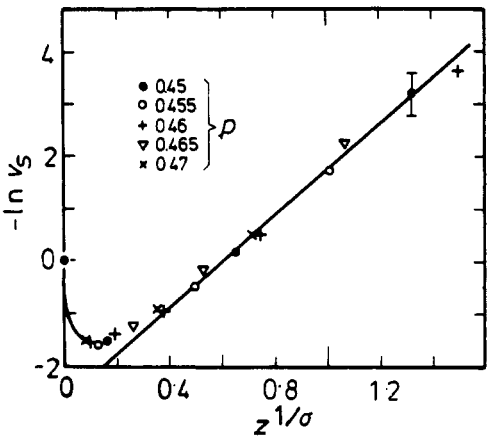

Figure 11. Test of scaling and asymptotic decay of cluster numbers below p_c. The straight-line fit suggests $\ln v_s \propto -s$ for large clusters, i.e. $\zeta = 1$.

data suggests that $\ln f(z) \propto -z^{1/\sigma}$, or for fixed p that $\ln v_s \propto -s$ for large s, which means

$$\zeta = 1. \tag{11}$$

Leath and Reich, using a different and more accurate analysis, also confirmed this simple result (11) and showed that the choice $\zeta = 2\sigma$ is not so good. $\zeta = 1{\cdot}1 \pm 0{\cdot}1$ was found also by Müller-Krumbhaar and Stoll (1976) for the square lattice at $p = \frac{1}{2}$, rather far below $p_c = 0{\cdot}59$, but with better statistics than our data below p_c. Thus conclusion (11) seems no longer controversial.

Müller-Krumbhaar and Stoll (1976) tried to fit the function $v_s(p)$ at $p = \frac{1}{2}$ in the square lattice over the whole range of s by $\ln v_s = -As + Bs^{\sigma}$. But now the constant B in this attempt is inconsistent with the value given by equation (7*a*), indicating the insufficiency of their simple *ansatz*.

Since that *ansatz* and also the simple Fisher model (Fisher 1967) with $\ln v_s \propto -s^{\sigma}$ above p_c have been shown to be inaccurate, we now look for other simple expressions for the scaling function $f = f(z)$ in equations (1) and (2). Figure 12 shows that the data for f on both sides of the phase transition follow roughly a parabolic ('Gaussian') curve on this semilogarithmic plot, just as was found also by Leath (1976), Wolff and Stauffer (1978), and Leath and Reich (1978). Closer inspection, however, indicates problems with this Gaussian fit. The full curve shown in the figure is given by the Gaussian

$$f(z) \simeq 5 \exp[-8{\cdot}7(z + 0{\cdot}4)^2], \tag{12a}$$

and gives reasonable overall agreement with the data but deviates systematically near $z = 0$. If the parabola were forced to fit better near $z = 0$ it would not fit the wings well. By inclusion of a cubic term the constraints $f_{\max} = 4{\cdot}9$ and $f(0) = 1$ can be maintained, and the overall fit improved somewhat. The broken curve in figure 12 represents the function

$$f(z) = \exp[-7{\cdot}1(z + z^2) + 1{\cdot}9z^3]. \tag{13a}$$

The slope $(\mathrm{d} \ln f/\mathrm{d}z)_{z=0}$ computed from equation (13*a*) has the value $-7{\cdot}1$, given in equation (7*a*), while the second derivative $(\mathrm{d}^2 \ln f/\mathrm{d}z^2)_{z=0}$ has the value $-14{\cdot}2$, comparable with the value -15 ± 1 given by equation (7*b*). $f_{\max} = 4{\cdot}9$ occurs at the

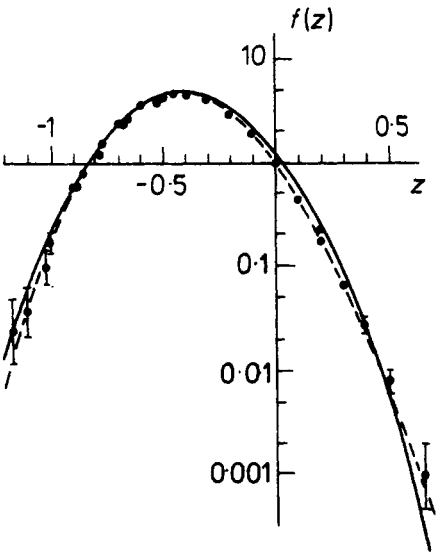

Figure 12. Logarithmic plot of $v_s = n_s(p)/n_s(p_c)$ below, at and above p_c as a function of $z = (p - p_c)s^{\sigma}$. The full curve is the parabola of equation (12); the broken curve is from equation (13) which includes a cubic correction term.

value $z_{max} = -0{\cdot}43$, comparable with that in equation (9). With the cluster numbers at p_c given by $n_s = q_0 s^{-\tau}$, the above expressions for $f(z)$ yield

$$n_s = 0{\cdot}15\, s^{-\tau} \exp\{-8{\cdot}7[(p - p_c)s^{\sigma} + 0{\cdot}4]^2\} \tag{12b}$$

and

$$n_s = 0{\cdot}18\, s^{-\tau} \exp\{-7{\cdot}1[(p - p_c)s^{\sigma} + 0{\cdot}5]^2 + 1{\cdot}9(p - p_c)^3 s^{3\sigma}\} \tag{13b}$$

respectively. These formulae can serve as valid approximations for z between about $-1{\cdot}3$ and $0{\cdot}6$, but not for the asymptotic decay or at larger $|z|$.

5. The exponents β and γ in two dimensions

The most accurate methods of determining the critical exponents β and γ are presumably Padé approximations to power series for these quantities (Sykes *et al* 1976) and the combination of renormalisation group theory with Monte Carlo analysis of large cells (Reynolds *et al* 1978). Fortunately both methods seem to give the same $\beta \approx 0{\cdot}138$ and $\gamma \approx 2{\cdot}43$ for the exponents of the 'spontaneous magnetisation' $P_\infty \propto (p - p_c)^{\beta}$ and 'susceptibility' $\chi \equiv \Sigma\, s^2 n_s \propto (p_c - p)^{-\gamma}$. (Here P_∞ is defined as the fraction of occupied sites which belong to the infinite network.) Now we show that our own Monte Carlo results are consistent with thse exponents, although presumably less accurate. Moreover, we want to evaluate the ratio of susceptibilities above and below p_c, which seems to be controversial (Sykes *et al* 1976, Wolff and Stauffer 1978, Hoshen *et al* 1979, Nakanishi and Stanley 1978).

In a finite lattice with free boundaries, the 'infinite' network is approximated by the largest cluster appearing in the Monte Carlo simulation; we omitted it in our previous analysis. Now figure 13 shows its relative importance; note that $P_\infty = \frac{1}{2}$ near $p = \frac{1}{2}$

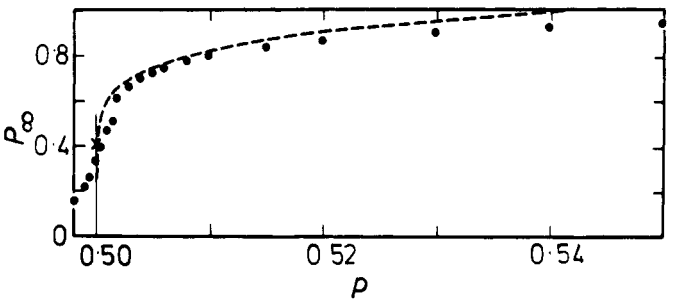

Figure 13. Percolation probability P_∞ (fraction of occupied sites belonging to largest cluster) as a function of p. The cross gives a result for a 2000×2000 lattice (Hoshen and Kopelman 1976), the full circles are for 4000×4000. The broken curve is the prediction of Sykes *et al* 1976: $P_\infty = B(p - p_c)^b$.

corresponds to a cluster of 4×10^6 sites, much larger than the largest cluster shown in figure 1. The broken curve in figure 13 corresponds to the series estimate $P_\infty = (1{\cdot}558 \pm 0{\cdot}002)(p - p_c)^{0{\cdot}138 \pm 0{\cdot}007}$ of Sykes *et al* (1976) and agrees reasonably, but not well, with our data. The influence of finite lattice sizes prevents us from determining β directly from this plot; for example, $P_\infty(p = p_c)$ does not vanish in our plot. Indeed, at $p = \frac{1}{2}$ a point for the 2000×2000 lattice gives an even larger value of $P_\infty(p_c)$.

Figure 14 shows the Monte Carlo susceptibility $\chi \equiv \Sigma s^2 n_s$ on both sides of p_c. Our sums for χ were evaluated from the groups of s between 2^i and 2^{i+1}, as explained at the beginning of § 2. The data on this log–log plot fall onto two straight lines corresponding to $\chi \propto (p - p_c)^{-2{\cdot}6}$ above p_c and $\chi \propto (p_c - p)^{-2{\cdot}2}$ below p_c. Scaling requires these two exponents to be the same; the observed deviations are again due to the finite lattice size

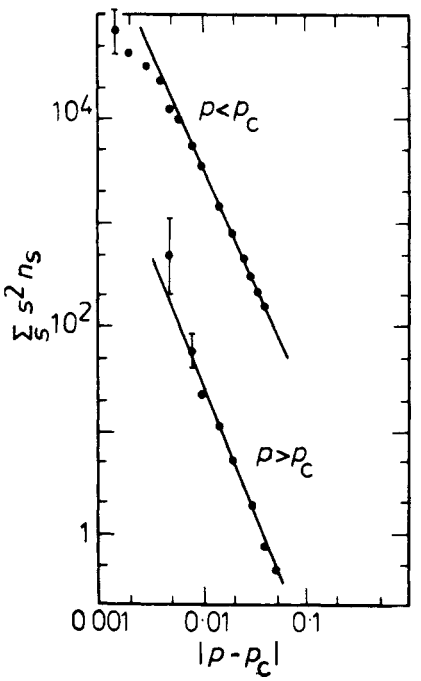

Figure 14. Log–log plot of the susceptibility $\chi \equiv \Sigma s^2 n_s$ as a function of $p - p_c$.

used here. (For size effects in percolation see Sur *et al* (1976), Levinshtein *et al* (1975), Roussenq *et al* 1976), Harrison *et al* (1978), Hoshen *et al* (1979); for size effects in magnets see Landau (1976), Müller-Krumbhaar (1978).

To extract more information in spite of the fact that we used only one lattice size here, we follow a suggestion of K Binder (private communication) and shift our apparent percolation threshold p_c^s upwards from the true $p_c = \frac{1}{2}$ until the two exponents for the susceptibility agree with each other. Using $0{\cdot}01 \leqslant |p - p_c| \leqslant 0{\cdot}05$ we found a symmetric exponent $\gamma \simeq 2{\cdot}36 \pm 0.10$ if p_c^s was taken as $0{\cdot}5008_5$:

$$\chi/p_c = 0.17(p_c^s - p)^{-2{\cdot}36} \text{ below } p_c, \tag{14a}$$

$$\chi/p_c = 0{\cdot}0009(p - p_c^s)^{-2{\cdot}36} \text{ above } p_c. \tag{14b}$$

The susceptibility amplitude ratio is given roughly by $0{\cdot}17/0{\cdot}009$, or

$$\chi_{p<p_c}/\chi_{p>p_c} = 196 \pm 40. \tag{14c}$$

The susceptibility amplitude below p_c agrees well with the series result (Sykes *et al* 1976) $\chi/p = 0{\cdot}13(p_c - p)^{-2{\cdot}43}$, and the ratio in equation (12*c*) agrees with the 'series' extrapolation of Wolff and Stauffer (1978) who give 180 ± 40. But a different series analysis of Sykes *et al* (1976) for the amplitude above p_c gave a ratio of only about 2; and Monte Carlo results of Hoshen *et al* (1979) and Nakanishi and Stanley (1978) gave ratios in between these extremely different estimates of about 2 and about 200.

But Sykes *et al* (1976) and also Nakanishi and Stanley (1978) actually looked at the quantity $S = \Sigma\, s^2 n_s / \Sigma\, s n_s = (1 - P_\infty)^{-1}\chi/p$, which is often called the mean cluster size and agrees only below p_c with the susceptibility χ_p. We have seen already that below p_c there is no disagreement with respect to the amplitudes. But above p_c the factor $(1 - P_\infty)^{-1}$ gives a correction term $1 + 0[(p - p_c)^\beta]$, which in two dimensions with β near $0{\cdot}14$ makes numerical extrapolations at finite values of $p - p_c$ very difficult. Our figure 13 shows how far away $1 - P_\infty$ is from its asymptotic value of unity. Indeed in our Monte Carlo work a log–log plot of S against $p - p_c$ (not shown) gave a much larger amplitude above p_c, leading to C_+/C_- near 20, in agreement ith Nakanishi and Stanley and at least closer to the series estimate of about 2. However, the exponent γ determined in this way for S above p_c had the unacceptably low value of $1{\cdot}9$, similar to the situation in the series result (Sykes *et al* 1976), where it was not possible to determine γ reliably above p_c. Thus it seems that above p_c the susceptibility $\Sigma\, s^2 n_s$ is more suitble than the mean cluster size $\Sigma\, s^2 n_s / \Sigma\, s n_s$ for extracting the asymptotic behaviour from series or Monte Carlo data; and the true ratio of amplitudes seems to be of order 10^2 and not of order unity.

The order of magnitude of our shift $p_c^s - p_c = 0{\cdot}00085$ agrees with general expectations (Levinshtein *et al* 1975, Roussenq *et al* 1976, Sur *et al* 1976, Hoshen *et al* 1978; Landau 1976, Müller-Krumbhaar 1979) that the shift should be proportional to $L^{-1/\nu}$ in a system with linear dimension L, where ν—here about $1{\cdot}35$: Reynolds *et al* (1978) with earlier literature, Klein *et al* (1978b)—is the exponent for the correlation length. For $L = 4000$ our shift of $0{\cdot}00085$ corresponds to a reasonable proportionality factor in that relation:

$$p_c^s(L) - p_c = 0{\cdot}39L^{-0{\cdot}74}. \tag{15}$$

With this apparently plausible shift of the critical point, we return to the 'spontaneous magnetisation' or percolation probability P_∞ of figure 13 and replot in figure 15 the same data double-logarithmically against $p - p_c^s$, with the same $p_c^s = 0{\cdot}00085$ as

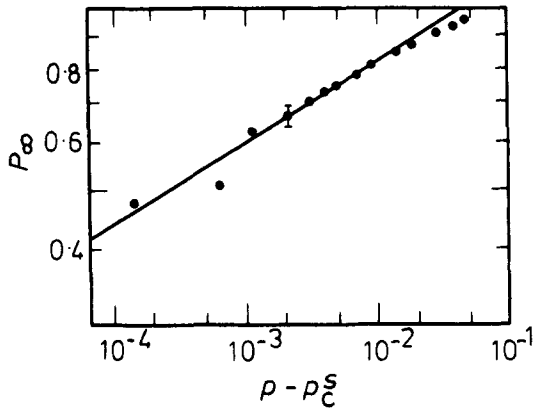

Figure 15. Log–log plot of P_∞ (same data as figure 13) when p_c is shifted to $p_c^s = 0.50085$, as determined from the susceptibilities. The full line has slope $\beta = 0.133$.

determined from the susceptibility. Now the data follow nicely a straight line for $p - p_c^s$ between 0·002 and 0·01, with

$$P_\infty = 1.5(p - p_c^s)^{0.133 \pm 0.01}. \tag{16}$$

The agreement of exponent and amplitude with the above-mentioned series result of Sykes *et al* (1976) is excellent. Thus even for these difficult data with a very small β we could get out the desired exponent by simply shifting the critical point such that the susceptibility exponent was symmetric about p_c. And our data for β and γ then do not contradict those we used right from the start to analyse our cluster numbers. We also note that a more complete investigation of critical exponents is in progress at the University of Michigan, based on a larger sample of lattices and using raw rather than grouped data.

Let us now return to the cluster numbers 'at p_c', figure 2. We have included in that plot also our data at $p = p_c^s$. Indeed these 'shifted' cluster numbers give a much better constant in figure 2 than the original data at $p = p_c = \frac{1}{2}$. On the other hand this shift is too small to affect the correction to scaling at small s (equations (5) and (6)). But of course this shifting of p_c is still only an approximation to incorporate size effects in the cluster numbers; no shift in p_c can given us cluster sizes s larger than the lattice size L^d, for example. A thorough study of size effects in the cluster numbers, using different lattice sizes L and different boundary conditions (see Landau (1976) for magnets), remains to be done.

If P_∞ and χ vanished and diverged respectively at two different critical points p_β and p_γ, then the relation $p_c = \frac{1}{2}$ of Sykes and Essam (1964) would no longer be valid and would be replaced by $p_\beta + p_\gamma = 1$ (Seymour and Welsh 1978). Our data suggest $|p_\beta - p_\gamma| < 10^{-3}$, in agreement with a recent, nearly exact result (Hintermann *et al* 1978) that the critical point in percolation is unique.

6. Three-dimensional results

In three dimensions we have results on both the simple cubic lattice and the BCC-1,2 lattice, affording an opportunity to test the universality concept as well as to make

analyses similar to those just described for the triangular lattice. Plots which summarise the cluster number data for the simple cubic $(100)^3$ and $(86)^3$ and the BCC-1,2 128000 site $2(40)^3$ lattices are given in figures 16(*a*), (*b*) and (*c*). These illustrate the degree to

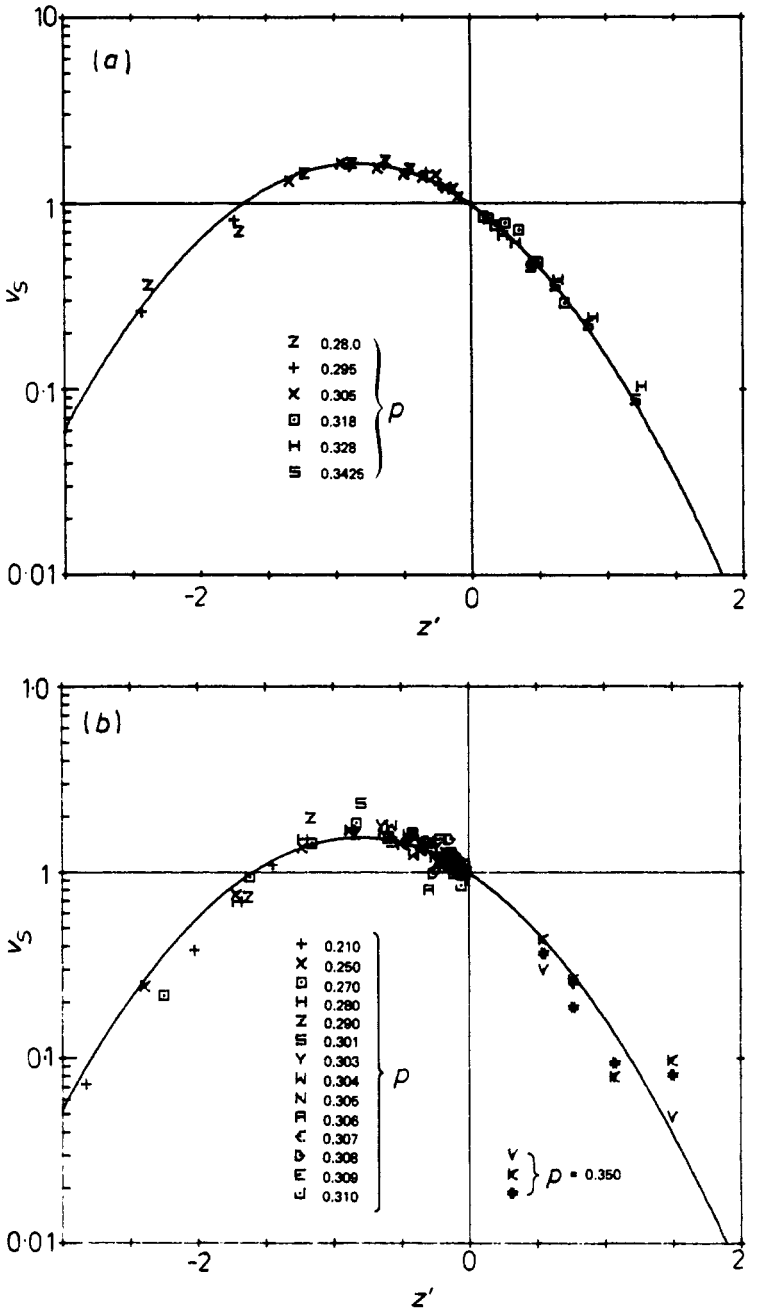

Figure 16. Logarithmic plot of $v_s = n_s(p)/n_s(p_c)$ below, at and above p_c as a function of $z' = (p/p_c - 1)s^{\sigma}$: (*a*) simple cubic $(100)^3$; (*b*) simple cubic $(86)^3$; (*c*) BCC-1,2 128000 sites $2(40)^3$. The curve in each figure is the same, i.e. equation (15).

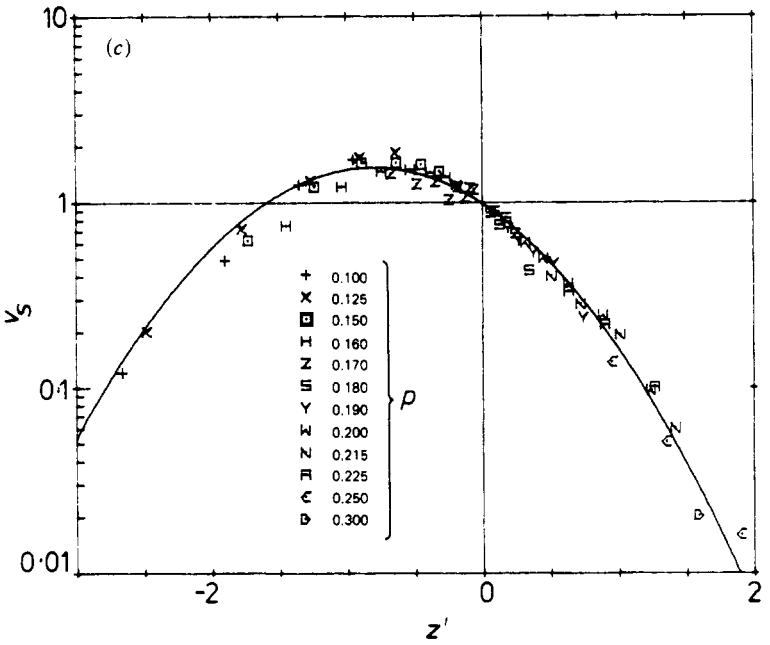

Figure 16. (Continued)

which the two-exponent scaling assumption of equation (1) as well as universality are satisfied. We have plotted on a logarithmic scale the variable $v_s = n_s(p)/n_s(p_c)$ as a function of the variable $z' \equiv z/p_c \equiv (p/p_c - 1)s^{\sigma}$, with the choice $\sigma = 0{\cdot}48$ consistent with the series results of Sykes *et al* (1976). On each of the figures we have also plotted a parabola $H[1-(z'/z'_{\max}-1)^2]$, where $H = \lg (v_s)_{\max}$, with $(v_s)_{\max}$ taken as 1·55 and $z'_{\max}$ taken as −0·792. These constants were chosen to provide a reasonable fit to all of the data and correspond to the approximation

$$f(z') \simeq 1{\cdot}55 \exp[-\ln 1{\cdot}55(z'/z'_{\max}-1)^2]. \tag{17}$$

The agreement shows that the universality concept is at least approximately satisfied. Constants which optimise the fit to the simple cubic $(100)^3$ data, which appear to be the most reliable, are $(v_s)_{\max} = 1{\cdot}63$ and $z'_{\max} = -0{\cdot}834$. The fit to the parabola is good, with no systematic deviations apparent within the range of the data; however, the same arguments cited for the triangular lattice suggest that the agreement must break down for larger values of $|z'|$, or that the deviations from scaling for larger values of $|p-p_c|$ may be important. The fact that σ is so close to $\frac{1}{2}$ in three dimensions would make the deviation at the larger $|z'|$ for negative values of z' smaller than for two dimensions, and this, combined with the fact that the range of z' extends more towards negative z', may be the reason why the parabolic fit appears so good. It is also striking that the value of $z'_{\max}$ is close to the value found for two dimensions. The value of $f_{\max} = (v_s)_{\max} \simeq 1{\cdot}6$ also agrees within statistical error with that obtained by plotting the individual values of n_s (figure 17), which gives $f_{\max} = 1{\cdot}56 \pm 0.09$. The kind of universality shown by the agreement between the FCC and BCC results has been discussed by Marro (1976) and Hoshen *et al* (1979), and our results verify that the use of the variable $z' = z/p_c$ brings the universality into evidence. Our new results fit nicely into the general picture of how percolation properties depend on the lattice dimensionality d. In one dimension the

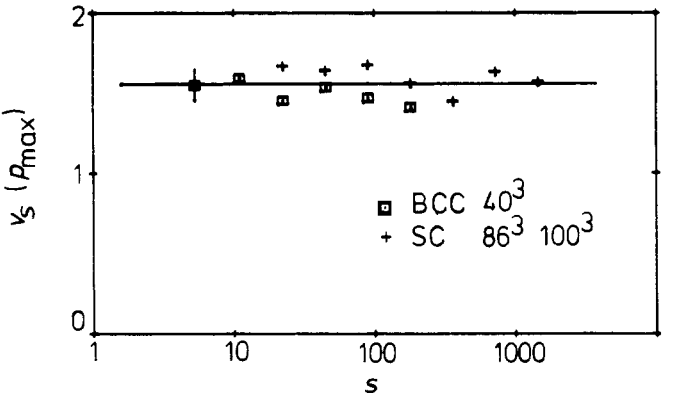

Figure 17. Maximum value of $n_s(p)/n_s(p_c) = v_s(p_{max})$ plotted against lg s. The line gives $f_{max} = 1{\cdot}56 \pm 0{\cdot}09$.

ratio f_{max} is infinite since $n_s(p_c)$ vanishes at $p = p_c = 1$, even if longer ranges of interaction (Klein *et al* 1978a) are used. In two dimensions triangular, square and honeycomb lattices gave the same $f_{max} \simeq 4{\cdot}5$ from extrapolation of exact results (Stauffer 1976), which is consistent with our present estimate of 4·9, but analogous attempts in three dimensions by Flammang (1977) were not successful in providing a reliable estimate of f_{max}. For infinite dimensionality one expects the Bethe lattice result $f_{max} = 1$ (Essam and Gwilym 1971).

The results we have to report on the $400 \times 400 \times 400$ simple cubic lattice are limited to a single random number starter for $0{\cdot}310 \leq p \leq 0{\cdot}314$. For our smaller three-dimensional lattices we used *periodic boundary conditions* in counting cluster numbers, whereas in the $(400)^3$ simple cubic lattice as well as for the $(4000)^2$ triangular lattice this was not done. One difference produced by the periodic boundary conditions is that the numbers of small clusters agree within statistical error with the numbers predicted by the cluster polynomials, whereas the deviations for the $(4000)^2$ and $(400)^3$, although small, are several times the statistical error. There is also an apparent effect in the value of p_c obtained with the different boundary conditions. For the simple cubic lattice our results for $(86)^3$ and $(100)^3$ are consistent with the value $p_c = 0{\cdot}3115$ also obtained by Sur *et al* (1976) and close to predictions of Sykes *et al* (1976) and Kirkpatrick (1976). For the $(400)^3$ lattice the results (see also Hoshen *et al* (1979) seem more consistent with the value $p_c = 0{\cdot}313$. Figure 18 shows the cluster numbers at $p = 0{\cdot}311$, together with the series prediction for p_c calculated from Gaunt (1977); the similarity to two dimensions, figure 1, is striking. But since the series prediction $\tau = 2{\cdot}20 \pm 0{\cdot}03$ is less accurate than in two dimensions, and since p_c is not known exactly, we made no attempt to find out the corrections to scaling as in equation (5*b*). Instead, assuming simply $n_s \propto s^{-\tau}$, with τ as a free parameter, we get $\tau = 2{\cdot}135 \pm 0{\cdot}008$ fitting to clusters larger than 64 and smaller than 16000. We have also obtained values of τ by fits to the cluster distribution at $p = 0{\cdot}312$ and 0·313, where we obtained best values of τ as 2·145 and 2·17 respectively. In addition to the quoted statistical error in evaluating the slopes, a change of the lower size cut-off from 64 to 256 produced a change of about 0·02 in τ. A similar study of the size distribution in the simple cubic $(100)^3$ lattice at $p = 0{\cdot}3115$ gave a best value $\tau = 2.16 \pm 0{\cdot}01$. The cluster distribution for the $(400)^3$ lattice at $p = 0{\cdot}314$ showed a single cluster an order of magnitude larger than the next smallest cluster, characteristic of the regime above p_c.

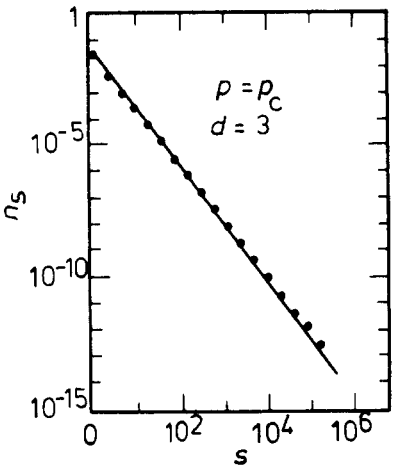

Figure 18. Variation of n_s with s at $p \cong p_c = 0{\cdot}311$ in a simple cubic $(400)^3$ lattice. The full line is the prediction of Gaunt (1977). See also figure 1.

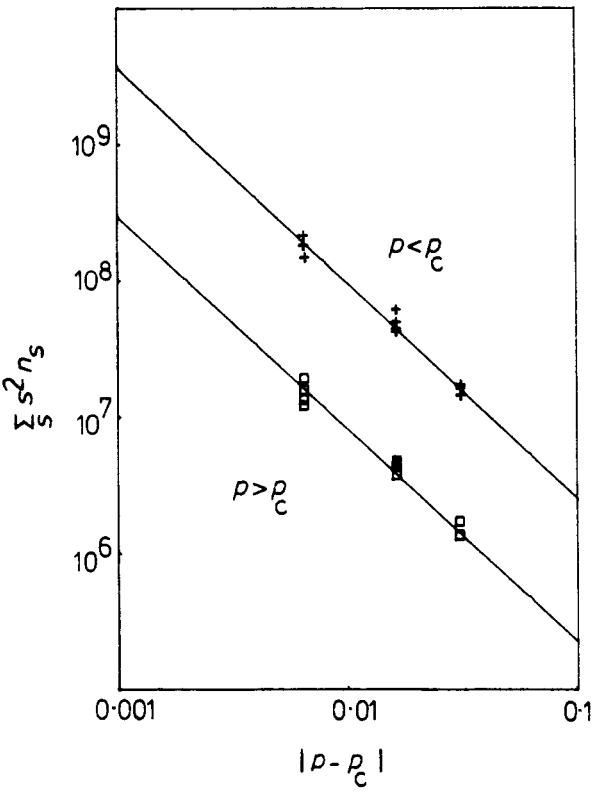

Figure 19. Log–log plot of the susceptibility $\chi \equiv \Sigma\, s^2 n_2$ as a function of $|p - p_c|$.

We have also examined the susceptibility $\chi = \Sigma\, s^2 n_s$ for the simple cubic $(100)^3$ lattice. Our analysis is somewhat different from that applied to the two-dimensional data, where the theoretical value of p_c was known and grouped data were used. We

have obtained the values of $\Sigma s^2 n_s$ by summing over individual clusters, counting the largest cluster, and of $\Sigma' s^2 n_s$, omitting the largest cluster. The values of these quantities at $p = 0{\cdot}3115$, the nominal value of p_c, are particularly interesting. For sums excluding the largest, the values fall into two groups differing by almost an order of magnitude. The smaller numbers correspond to those samplings which look super-critical; that is, the largest cluster is much larger than its nearest competitors. One expects this sort of behaviour in a finite sample. Accordingly we have plotted the data above and below p_c not only against $|p - p_c|$, testing various choices of p_c, but also (as in Harrison *et al* 1978) against $[(p-p_c)^2 + W^2]^{1/2}$, taking $W = 0{\cdot}0025$, a value obtained by extrapolating results of Levinshtein. The values of γ estimated (assuming $p_c = 0{\cdot}3115$) from the sums for $p > p_c$ and for $p < p_c$ agree to within probable error, for choice $W = 0$ and the data at $p = 0{\cdot}3115$ omitted of necessity from the fit. The data are plotted in figure 19. (The slopes above and below p_c would agree exactly with the choice $p = 0{\cdot}3114$, with γ then equal to 1·56.) With W chosen equal to 0·0025 one obtains the values for γ from p above and below p_c of 1·61 and 1·63 respectively, with p_c chosen as 0·3115. When $W \neq 0$ one has the choice either of including or excluding the values obtained at the nominal p_c. We have plotted in figure 20 the values of $\Sigma s^2 n_s$ and of $\Sigma' s^2 n_s$, including the values at 0·3115 both with and without the largest cluster. The lines drawn are fitted

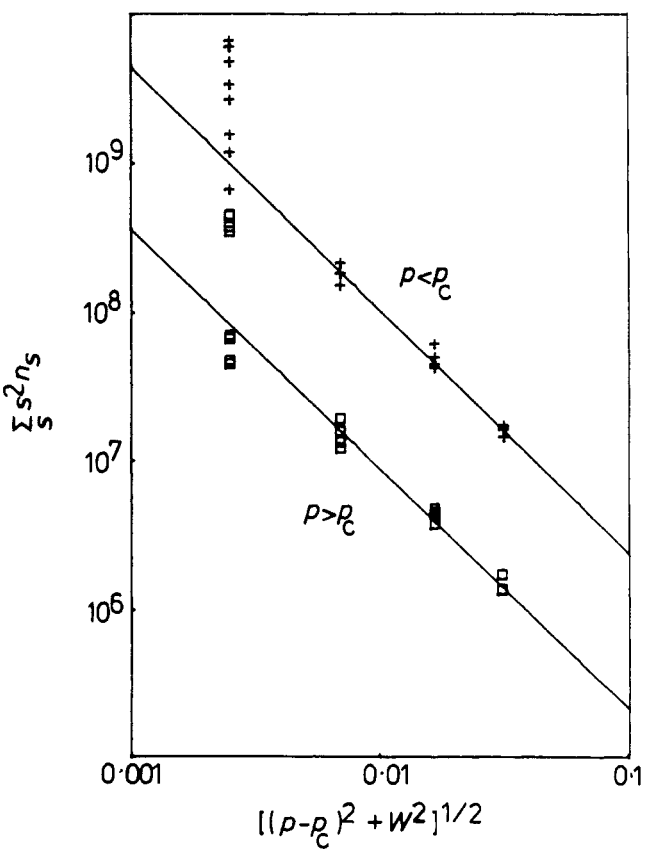

Figure 20. Log–log plot of the susceptibility $\chi \equiv \Sigma s^2 n_s$ as a function of $[(p-p_c)^2 + W^2]^{1/2}$, for $W = 0{\cdot}0025$.

without considering this point, but it is interesting that the data right at p_c appear to fit quite reasonably. The bimodal distribution mentioned above for $p = 0{\cdot}3115$ may be an accident of the statistical method, however, the width of the critical concentration region given by the value of W indicates one may easily have samples which contain a 'slice of the infinite cluster' and those that do not. The susceptibility amplitude ratio for the simple cubic lattice obtained for $W = 0$ is approximately 11. (It does not change significantly for $W \neq 0$.) About the same value is also obtained for the BCC–1,2 lattice.

7. Conclusions

This paper confirms the following: In both two and three dimensions the cluster numbers follow the two-exponent scaling assumption (1); in two dimensions the decay of n_s for large clusters is as $\ln n_s \propto -s$ below p_c and as $\ln n_s \propto s^{1/2}$ above p_c, starting fairly close to p_c. This is consistent with the work of Stoll and Domb (1978), Leath and Reich (1978) and Nakanishi and Stanley (1978). Moreover, we obtained cluster numbers at the critical point over many orders of magnitude in the cluster size and analysed corrections to scaling. The ratio of susceptibilities below and above p_c was determined to be about 200 in two dimensions and about 11 in three dimensions. The ratio of cluster numbers $n_s(p)/n_s(p_c)$ reaches a maximum of about 5 in two dimensions and about 1·6 in three dimensions. This maximum value is reached at approximately the same value of $(p/p_c - 1)s^{\sigma} \simeq -0{\cdot}8$ in two and in three dimensions. In two dimensions the data on $n_s(p)/n_s(p_c)$ show asymmetrical distortions with respect to the approximate Gaussian fit which can be represented over the range of the data by a cubic term. In three dimensions the Gaussian fit itself is fairly good.

The asymmetry of the Kunz–Souillard exponents about p_c which we confirmed here suggests a difference in the structure of clusters above and below p_c, since a 'surface' exponent $1 - 1/d$ appears only above and not below p_c. Monte Carlo calculations of cluster structures above and below p_c have also been made (Leath 1976, Domb and Stoll 1977, Domb 1978, Leath and Reich 1978, Stoll and Domb 1978, Stauffer 1978) together with analytic arguments (Stauffer 1976, Hankey 1978). The discussion of these results is beyond the scope of the present paper.

Acknowledgments

We appreciate suggestions and discussion with K Binder, C Domb, W Klein, J L Lebowitz, H Müller-Krumbhaar, H Nakanishi and H E Stanley. DS wishes especially to thank H E Stanley for repeated hospitality at Boston University. GHB, RJH and GJQ recall that last fall C Domb urged them to compare their Monte Carlo Data with the scaling assumption of equation (1) and only belatedly acted on this suggestion after the recent visit of DS and JH to Boston University where the authors' collaboration was set up. JH also wishes to thank Paul Klymko and Raoul Kopelman for collaborative efforts on the cluster distribution, and The University of Michigan for computing funds.

Note added in proof. Further information on cluster numbers will be given by Stoll and Domb (1979).

References

Amit D J 1976 *J. Phys. A: Math. Gen.* **9** 1441–59
Bakri M and Stauffer D 1976 *Phys. Rev.* B **14** 4215–8
Bauchspiess K R and Stauffer D 1978 *J. Aerosol Sci.* **9** 567–77
Binder K and Müller-Krumbhaar H 1974 *Phys. Rev.* B **9** 2328–53
Domb C 1974 *J. Phys. C: Solid St. Phys.* **7** 2677–80
—— 1976 *J. Phys. A: Math. Gen.* **9** L141–8
—— 1978 *Ann. Isr. Phys. Soc.* vol. 2 *Statistical Physics–STATPHYS 13* (Bristol and Haifa: Adam Hilger and The Israeli Physical Society) pp 61–74
Domb C and Pearce C J 1976 *J. Phys. A: Math. Gen.* **9** L137–40
Domb C and Stoll E 1977 *J. Phys. A: Math. Gen.* **10** 1141–9
Essam J W 1972 *Phase Transitions and Critical Phenomena* vol. 2, ed. C Domb and M S Green (London and New York: Academic) pp 197–270
Essam J W and Gwilym K M 1971 *J. Phys. C: Solid St. Phys.* **4** L228–32
Fisher M E 1967 *Physica* **3** 255–83
Flammang A 1977 *Z. Phys.* B **28** 47–50
Gaunt D S 1977 *J. Phys. A: Math. Gen.* **10** 807–12
Gaunt D S and Sykes M F 1976 *J. Phys. A: Math. Gen.* **9** 1109–16
Hankey A 1978 *J. Phys. A: Math. Gen.* **11** L49–55
Harrison R J, Bishop G H and Quinn G D 1978 *J. Stat. Phys.* **19** 53–64
Hintermann A, Kunz H and Wu F Y 1978 *J. Stat. Phys.* **19** 623–32
Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438–45
Hoshen J, Kopelman R and Monberg E M 1978 *J. Stat. Phys.* **19** 219–42
Houghton A, Reeve J S and Wallace D J 1978 *Phys. Rev.* B **17** 2956–65
Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574–88
—— 1976 *Phys. Rev. Lett.* **36** 69–72
Klein W, Stanley H E, Redner S and Reynolds P J 1978a *J. Phys. A: Math. Gen.* **11** L17–22
Klein W, Stanley H E, Reynolds P J and Coniglio A 1978b *Phys. Rev. Lett.* **41** 1145–8
Kunz H and Payandeh B 1978 *Preprint*
Kunz H and Souillard B 1978 *Phys. Rev. Lett.* **40** 133–5; *J. Stat. Phys.* **19** 77–106
Landau D P 1976 *Phys. Rev.* B **13** 2997–3011; *Phys. Rev.* B **14** 255–62
Leath P L 1976 *Phys. Rev.* B **14** 5046–55
Leath P L and Reich G R 1978 *J. Phys. C: Solid St. Phys.* **11** 4017–36
Levinshtein M E, Shklovskii B I, Shur M S and Efros A L 1975 *Zh. Eksp. Teor. Fiz.* **69** 386–92 (Engl. Transl. *Sov. Phys.-JETP* **42** 197–9)
Marro J 1976 *Phys. Lett.* A **59** 180–1
Müller-Krumbhaar H 1978 *Monte Carlo Methods in Statistical Physics* ed. K Binder (Berlin: Springer) ch 5
Müller-Krumbhaar H and Stoll E 1976 *J. Chem. Phys.* **65** 4294–302
Nakanishi H and Stanley H E 1978 *J. Phys. A: Math. Gen.* **11** L189–97
Priest R G and Lubensky T C 1976 *Phys. Rev.* B **13** 4159–71; *Phys. Rev.* B **14** 5125 (erratum)
Quinn G D, Bishop G H and Harrison R J 1976a, *J. Phys. A: Math. Gen.* **9** L9–14
—— 1976b *Nucl. Metal.* **20** 1213–25
Reynolds P J, Stanley H E and Klein W 1978 *J. Phys. A: Math. Gen.* **11** L199–207
Roussenq J, Clerc J, Giraud G, Guyon E and Ottavi H 1976 *J. Physique* **37**, L99–100
Seymour P D and Welsh D J A 1978 *Advances in Graph Theory, Annals of Discrete Mathematics* No 3, ed. B Bollobas (Amsterdam: North-Holland)
Stauffer D 1975 *Phys. Rev. Lett.* **35** 394–7
—— 1976 *Z. Phys.* B **25** 391–9
—— 1978 *Preprint*; see also *J. Stat. Phys.* **18** 125–36
Stephen M J 1977 *Phys. Rev.* B **15** 5674–80
Stoll E, Binder K and Schneider T 1972 *Phys. Rev.* B **6** 2777–80
Stoll E and Domb C 1978 *J. Phys. A: Math. Gen.* **11** L57–61
—— 1979 *J. Phys. A: Math. Gen.* at press
Sur A, Lebowitz J L, Marro J, Kalos M H and Kirkpatrick S 1976 *J. Stat. Phys.* **15** 345–53
Sykes M F and Essam J W 1964 *J. Math. Phys.* **5** 1117–27
Sykes M F, Gaunt D S and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 97–103, 715–24, 725–30
Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87–95
Wolff W F and Stauffer D 1978 *Z. Phys.* B **29** 67–9