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Percolation in two-dimensional lattices

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Abstract. Using a definition of percolation suitable for finite lattices we closely examine the percolation of such lattices. By extrapolation we can calculate accurate values for the critical density p_c and discuss the size dependence of percolation. With the aid of a computer we enumerate exactly a certain class of site percolation configurations of finite square lattices with up to 81 sites. Rapidly convergent extrapolation procedures allow accurate determination of the critical density for percolation of the corresponding infinite lattice. We find $p_c = 0.5898 \pm 0.0008$ for the site problem on a square lattice.

1. Introduction

No general theory exists for determining the critical parameters for percolation on lattices (for a review see Shante and Kirkpatrick 1971). Theoretical progress has depended on accidental symmetries which allow calculations for some special lattices (Fisher and Essam 1961) and on numerical methods. In certain two-dimensional cases Sykes and Essam (1963, 1964a) have been able to establish a matching property for pairs of lattices. With the help of symmetries this approach leads to a few exact solutions for the critical density p_c . The most important approximate methods are the series expansion method (Sykes and Essam 1964b) which yields results accurate, with moderate effort, to a few percent, and the Monte Carlo method (Dean 1963, Frisch *et al* 1961, Vyssotsky *et al* 1961) which yields similar precision.

In this paper we take a somewhat different approach to the problem. We consider site percolation through two-dimensional $N \times N$ lattices and we treat them exactly, extrapolating to arrive at the infinite-system result (see also Imry and Bergman 1971). We say that a finite lattice percolates if there is a path across it from a selected edge to the opposite one. In this way most of the matching properties of Sykes and Essam (1963, 1964a) are trivial. In particular, consider the site problems on the square lattice and the square lattice with second neighbours included, to which cases our actual numerical work is limited. If there is a percolating path composed of empty sites in the horizontal direction according to the latter rule (percolation via first and second neighbours), there can be no percolating path composed of occupied sites in the vertical direction according to the former rule (percolation via nearest neighbours only). The converse also holds. Therefore, in the $N \rightarrow \infty$ limit the corresponding critical densities add to exactly one. We rely heavily on this property in our calculations. For technical reasons the problems we treat exactly are not quite the two site problems on a square lattice with first neighbours only and with first- and second-nearest neighbours included. The

some other possible definitions. (A 'possible' definition is one which reduces in the $N \rightarrow \infty$ limit to the statement that there exists an infinite connected cluster.)

We have calculated P_N exactly (subject to the restriction concerning the 'snakes' as mentioned in the introduction and discussed later in this section) for $N = 2, 3, \dots, 8$, which is sufficient to allow reliable extrapolation to $N = \infty$ (see § 4).

The function $P_N(p)$ has the form shown in figure 2. We plot P_N for $N = 1, 2, 3, 4, 6$. The limiting form of P_N for $N \rightarrow \infty$ is a θ -function:

$$P_\infty(p) = \theta(p - p_c) \tag{1}$$

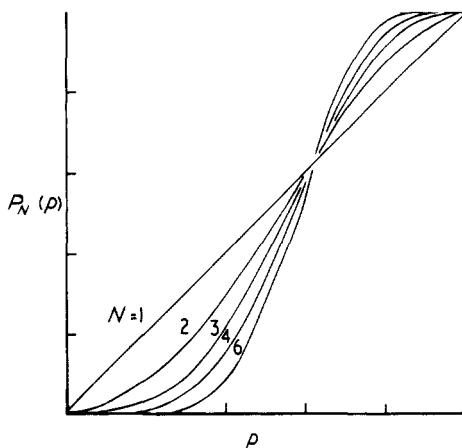


Figure 2. Percolation probability $P_N(p)$ as a function of p for $N \times N$ square lattices and $N = 1, 2, \dots, 6$.

where p_c is the critical percolation density. The behaviour of the P_N immediately suggests a number of extrapolation procedures which will yield a sequence p_{cN} which converges to p_c , for example, the solutions of

$$d^2 P_N(p)/dp^2 = 0 \tag{2}$$

or

$$P_N(p) = p. \tag{3}$$

Equation (3) is the result of a scaling approach and, incidentally, gives a surprisingly good estimate for the critical density, $p_c \approx 0.62$, already at $N = 2$.

We tried other schemes as well, more or less rapidly convergent. None could beat, however, the most straightforward possible definition for p_{cN} :

$$p_{cN} = 1 - N^{-2} \sum_{n=1}^{N^2-1} \mu_n^{(N)} \tag{4}$$

where $\mu_n^{(N)}$ is defined to be the percolating fraction of all configurations with precisely n occupied sites. Imagine filling randomly, one by one, the sites of an $N \times N$ lattice. The lattice will suddenly percolate when some number of sites n_S have been filled; p_{cN} , according to definition (4), is the mean value of n_S/N^2 . To see this, define the total number

of percolating configurations for occupation number n as

$$k_n^{(N)} = \binom{N^2}{n} \mu_n^{(N)}. \tag{5}$$

Now the number of random fillings of $n - 1$ sites which percolate is $(n - 1)! k_{n-1}^{(N)}$. Thus of the $n! k_n^{(N)}$ percolating fillings of n sites, $(N^2 - n + 1)(n - 1)! k_{n-1}^{(N)}$ already percolated when site $n - 1$ was filled. Hence

$$[n! k_n^{(N)} - (N^2 - n + 1)(n - 1)! k_{n-1}^{(N)}] / n! \binom{N^2}{n} = \mu_n^{(N)} - \mu_{n-1}^{(N)} \tag{6}$$

is the fraction of random fillings which percolate exactly when the n th site is filled. Therefore,

$$p_{cN} = N^{-2} \sum_n n(\mu_n^{(N)} - \mu_{n-1}^{(N)}) \tag{7}$$

and equation (4) follows from a summation by parts.

Prescription (4) is rapidly convergent ; our analysis (§ 4) indicates that the convergence is exponential with $p_{cN} - p_{c\infty} \sim e^{-\alpha N}$ and α approximately equal to unity. We find $p_{c\infty} = 0.5907 \pm 0.0001$.

The excellence of this last result is illusory, however, because the snakes are not included. Precisely defined, a snake is a configuration which includes a backwards string of occupied sites essential for percolation. The simplest kind of snake is shown in figure 3(a). The configuration in figure 3(b) is not a snake since there is a direct path available as well as the snake-like path. Snakes are rare (there are none at all for $N < 5$; less than one in 10^4 is a snake for $N = 5$) and make only a small contribution to percolation except in the very near vicinity of p_c . They are important, however, for an estimate of p_c which claims a precision better than 10^{-3} .

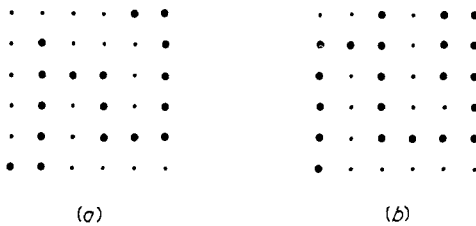


Figure 3. Configurations on 6×6 lattices: (a) is a snake; (b), although it has a snakey portion, is not.

The effect of omitting the snakes is that we overestimate p_c . Also the prescription (4) gives a sequence of decreasing upper bounds on p_c (reflecting the notion that larger systems percolate sooner than small ones). The result quoted above should therefore be considered only as an upper limit on p_c which we denote by $p_{c\infty}$. It is difficult to calculate directly the contribution of the snakes, but it is easy to generate a sequence of lower bounds. This leads us to the problem of first and second neighbours. As mentioned in the introduction, in order for a configuration *not* to percolate according to our definition, there must be a connected string of unoccupied sites blocking the way. The ‘connections’ between unoccupied sites follow a definite rule, but a different one from the rule for occupied sites ; in the case of the square lattice the complementary rule corresponds to percolation between nearest neighbours and second-nearest neighbours. The critical

percolation density \bar{p}_c for the latter percolation problem is clearly related to p_c by

$$\bar{p}_c = 1 - p_c. \quad (8)$$

Just as in the original problem, we can calculate \bar{P}_N and a sequence \bar{p}_{cN} which converges from above to a value slightly larger (because we again neglect the snake configurations) than \bar{p}_c . But because of (8) the sequence $\bar{q}_{cN} = 1 - \bar{p}_{cN}$ will bound the critical density for the first-neighbour problem from below.

In order to extrapolate for $\bar{q}_{c\infty}$ we will consider a procedure slightly different from equation (4). Equation (4) is the average of the critical proportion of sites that actually have to be occupied for percolation to take place in the microcanonical ensemble where the number of occupied sites is the relevant variable. One can also look at the problem in the canonical ensemble where the probability of occupation of a site is the relevant variable. One then gets for p_{cN} :

$$p_{cN} = 1 - \frac{1}{N^2 + 1} \sum_{n=0}^{N^2} \mu_n^{(N)} \quad (9)$$

which is strictly equivalent to equation (4) in the limit of large N . We derive equation (9) in the appendix where we discuss the question of ensembles at some length.

It turns out that the sequence p_{cN} as defined in equation (9) converges faster in the case of the first- and second-nearest neighbours than the one defined in equation (4), whereas the opposite is true for the first-neighbours-only case (all these sequences are given in table 1). On carrying out the indicated calculations we find, extrapolating as before from data for $N = 2, 3, \dots, 9$, that

$$0.5821 < p_c < 0.5907, \quad (10a)$$

the precision of the lower limit being ± 0.0014 . The values of \bar{p}_{c9} and p_{c8} both from equation (4) provide less sharp but precisely determined limits:

$$0.578 < p_c < 0.5908. \quad (10b)$$

The latter limits are firm since the microcanonical method of determining p_{cN} always reflects the fact that large systems percolate easier than small systems (Pike and Seager 1974).

Up to this point there is no other approximation in our approach than the extrapolation to $N \rightarrow \infty$. To improve the estimate for p_c we will have to evaluate the relative

Table 1. Sequences of percolation thresholds p_{cN} for the square lattice according to two definitions. The entries \bar{p}_{cN} are for percolation with connections to first- and second-nearest neighbours.

N	p_{cN} (equation 4)	\bar{p}_{cN} (equation 4)	p_{cN} (equation 9)	\bar{p}_{cN} (equation 9)	$\frac{1}{N^2 + 1} \sum_{n=0}^{N^2} (\mu_{\text{snake}}^{(N)} + \bar{\mu}_{\text{snake}}^{(N)})$
2	0.666667	0.583333	0.533333	0.466667	0.0
3	0.613757	0.497354	0.552383	0.447619	0.0
4	0.599260	0.463287	0.564009	0.436035	0.000044
5	0.594002	0.446257	0.571156	0.429093	0.00025
6	0.591895	0.436546	0.575898	0.424747	0.00065
7	0.591061	0.430577	0.579240	0.421966	0.00121
8	0.590809	0.426738	0.581720	0.420173	0.00189
9		0.424204		0.419031	

contributions of two different classes of snakes, namely those belonging to the two different problems respectively. The true p_c divides the small gap between $\bar{q}_{c\infty}$ and $p_{c\infty}$. For $p_c < p < p_{c\infty}$ and in the limit of large N , all percolation is via snakes. This statement can be formalized as follows. Define $\mu_{\text{snake}}^{(N)}(p)$ for $p = n/N^2$ as the fraction of all configurations with n occupied sites which percolate and which are snakes. Then as $N \rightarrow \infty$, $\mu_{\text{snake}}^{(N)}$ converges to

$$\mu_{\text{snake}}^{(\infty)} = \theta(p - p_c)\theta(p_{c\infty} - p). \tag{11}$$

For finite N , $\mu_{\text{snake}}^{(N)}$ is a broadened peak centred near p_c . For N less than a few hundred, the width of this peak is much greater than $p_{c\infty} - p_c$, in the same way as the μ_n for small N show no abrupt threshold at p_{cN} . We define similarly $\bar{\mu}_{\text{snake}}^{(N)}(p)$ which is the fraction of percolating snakes according to the complementary rule. Remarks analogous to those above apply to the function $\bar{\mu}_{\text{snake}}^{(N)}$, eg for $\bar{q}_{c\infty} < p < p_c$ all blocking strings of unoccupied sites are snakes in the limit $N \rightarrow \infty$. The functions $\mu_{\text{snake}}^{(N)}$ and $\bar{\mu}_{\text{snake}}^{(N)}$ are shown schematically in figure 4.

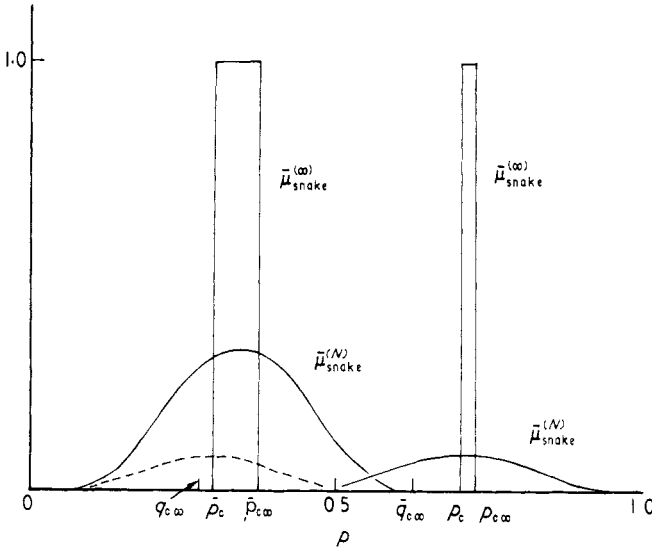


Figure 4. Schematic plot of the fractional number of snake configurations as a function of p . The bell-shaped curves would correspond to $N \sim 10$. The broken curve is the mirror image (about $p = 0.5$) of $\mu_{\text{snake}}^{(N)}$. The widths of $\mu_{\text{snake}}^{(\infty)}$ and $\bar{\mu}_{\text{snake}}^{(\infty)}$ are exaggerated as is the displacement of the centres of the broken peak and $\bar{\mu}_{\text{snake}}^{(N)}$. The p axis benchmarks are defined in the text.

There is an essential difference between the snakes that compose the families $\mu_{\text{snake}}^{(N)}$ and $\bar{\mu}_{\text{snake}}^{(N)}$. The simplest snakes of the two families are shown in figure 5. ‘Simplest’ here means configurations in which the percolation path is as short as possible. If the second-nearest neighbours are allowed to interact, as in figure 5(b), the snake configuration is a great deal simpler than the one seen in figure 5(a). We will call the former type uncomplicated as compared with the complicated snakes composing the family belonging to the first-neighbours-only problem.

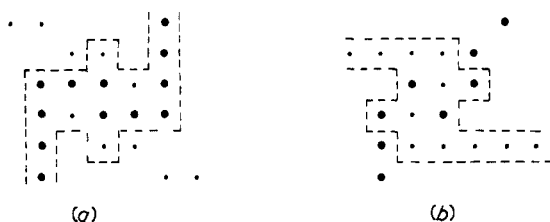


Figure 5. Simplest snake configurations for complementary connection rules. Occupancy of the sites within the broken lines must be as shown. Sites outside the broken lines are shown occupied in one of a class of equivalent ways.

The basis of our estimations of how the gap is to be divided between these two families of snakes is the assumption that their relative weights (their actual contributions to p_c and \bar{p}_c).

$$\frac{1}{N^2 + 1} \sum_{n=0}^{N^2} \mu_{\text{snake}}^{(N)} \quad \text{and} \quad \frac{1}{N^2 + 1} \sum_{n=0}^{N^2} \bar{\mu}_{\text{snake}}^{(N)}, \tag{12}$$

do not change too dramatically as a function of N after the snakes have made their appearances on the scene at $N = 4$ and $N = 5$. This is analogous with the fact that the critical points p_{cN} and \bar{p}_{cN} do not change much as functions of N . Then the ratio γ of the weights of the two families will be fixed at a relatively early stage in N . We have two different ways of estimating this ratio which one intuitively expects to be heavily in favour of the uncomplicated snakes.

As long as the peaks $\mu_{\text{snake}}^{(N)}$ and $\bar{\mu}_{\text{snake}}^{(N)}$ are much wider than the gap between $\bar{q}_{c\infty}$ and $p_{c\infty}$ and roughly equally wide, one can say that the ratio of the quantities in (12) is approximately equal to the ratio of the grand totals of snake configurations in the two families,

$$\eta_{\text{snake}}^{(N)} = \sum_{n=1}^{N^2} \binom{N^2}{n} \mu_{\text{snake}}^{(N)} (n/N^2) \tag{13}$$

and analogously for $\bar{\eta}_{\text{snake}}^{(N)}$. This is so as the binary coefficients then will not be very different for the two peaks. The necessary conditions are clearly met for $N = 5$, for which we have an explicit count of the snakes, and seem to remain satisfied at least up to $N = 8$.

Now it is possible for $N \leq 8$ to estimate in a simple way $\eta_{\text{snake}}^{(N)}$ and $\bar{\eta}_{\text{snake}}^{(N)}$, and hence γ . An $N \times N$ lattice admits of 2^{N^2} configurations altogether. To obtain a snake certain sites have to be occupied in a particular way as shown in figure 5. Suppose $\eta_{\text{snake}}^{(N)}$ and $\bar{\eta}_{\text{snake}}^{(N)}$ comprise chiefly such simple snakes. The sites shown within the broken lines must be occupied as indicated. In figure 5(a) the occupation of $2N + 9$ sites is specified, which reduces the number of snake candidates by a factor 2^{2N+9} . The corresponding factor in figure 5(b) is 2^{2N+6} . On this basis alone one would conclude that

$$\gamma = \bar{\eta}_{\text{snake}}^{(N)} / \eta_{\text{snake}}^{(N)} = 2^{N^2 - (2N+6)} / 2^{N^2 - (2N+9)} = 8. \tag{14}$$

Additionally there must be strings of filled (empty) sites as indicated in figure 5(b) ((a)), which can be positioned in a variety of ways (the remaining sites can be occupied or not in an arbitrary manner). Consideration of the possibilities shows that γ should be slightly increased over (14). The multiplicity of positionings of the snake figure is of

order N^2 , only a pre-exponential factor in (14), which, however, again favours an increased γ .

What about our assumption that the snakes of figure 5 exhaust $\eta_{\text{snake}}^{(N)}$ and $\bar{\eta}_{\text{snake}}^{(N)}$? First of all, more elaborate snakes require the rigid specification of more sites; secondly, the positional multiplicities of such snakes are smaller; thirdly, by actual count, at least the simpler elaborations contribute equally to $\eta_{\text{snake}}^{(N)}$ and $\bar{\eta}_{\text{snake}}^{(N)}$ leaving the ratio unaffected.

The above estimate of γ depends crucially upon the smallness of the gap $p_{c\infty} - \bar{q}_{c\infty}$, which results in the approximate proportionality of $\mu_{\text{snake}}^{(N)}$ and $\bar{\mu}_{\text{snake}}^{(N)}$ for small N , and upon the rapid convergence of the p_{cN} and \bar{p}_{cN} . We may thus extract γ from considerations of the snake population on low-order ($N \lesssim 8$) lattices. Only for low-order lattices can we enumerate with confidence the contributions of the various types of snake configurations.

Another and independent way of estimating the respective weights of the two families of snakes is starting with the explicit count of snakes at $N = 5$. There the ratio of the relative weights (12) is $\gamma = 26$ in favour of the uncomplicated type (the ones of the first-and-second-neighbour case). In table 1 we also give the sum of the quantities (12) (ie the contributions of all snakes) for $N = 1, 2 \dots 8$. One can see that the effective share of the snakes grows rapidly after $N = 4$ and its value would be the width of the gap at $N = \infty$. The obvious reason for the reduced weight of the snakes for small N is the finite size of a snake configuration. There is no room for the uncomplicated type for $N < 4$ and the complicated type for $N < 5$. The rapid growth after $N = 4$ reflects the relaxing of the space problem. There is a phase lag of unity between the uncomplicated and the complicated snakes with respect to the increasing room, and one would therefore expect the share of the complicated snakes to grow.

To obtain a quantitative estimate of this we will call $a_{N,N+1}$ the ratios of the contributions of snakes for two consecutive values of N . Then $a_{4,5} = 0.00025/0.000044 = 5.7$ (table 1), $a_{5,6} = 2.6$ etc. As at $N = 5$ still only $1/27$ of the snakes are of the complicated type, $a_{4,5}$ mainly describes the growth of the share of the uncomplicated snakes from the minimum space of 4×4 to 5×5 . In the 5×5 lattice the uncomplicated snakes have room for expansion in two dimensions, each presumably contributing a factor $\sqrt{a_{4,5}}$ compared with 4×4 . From $N = 5$ to $N = 6$ as well, each spatial direction is expected to contribute a factor $\sqrt{a_{5,6}}$. The complicated type of snake requires a minimum space 4×5 . Thus the growth from the lattice 5×5 to 6×6 includes one factor $\sqrt{a_{5,6}}$ and one $\sqrt{a_{4,5}}$, the latter describing the growth from the entirely constrained horizontal direction in $N = 5$ to one step of leeway in $N = 6$, just as was the case of the uncomplicated snakes in both directions from 4×4 to 5×5 . The coefficients for going from $N = 6$ to $N = 7$ etc can be constructed analogously leading to the ratio γ at $N = \infty$ (remembering that the $a_{N,N+1}$ tend to unity for large N):

$$\gamma = 26 \frac{a_{5,6}}{\sqrt{a_{5,6}}\sqrt{a_{4,5}}} \frac{a_{6,7}}{\sqrt{a_{5,6}}\sqrt{a_{6,7}}} \frac{a_{7,8}}{\sqrt{a_{6,7}}\sqrt{a_{7,8}}} \dots = \frac{26}{\sqrt{a_{4,5}}} \simeq 11. \tag{15}$$

Thus both of our estimations roughly agree and we conclude that $\gamma \sim 10$ which implies that p_c is about ten times closer to $p_{c\infty}$ than $\bar{q}_{c\infty}$. Taking generously $6 < \gamma < 26$ (26 is the ratio at $N = 5$) and allowing for the stated error limits in $p_{c\infty}$ and $\bar{q}_{c\infty}$, we arrive at our final result,

$$p_c = 0.5898 \pm 0.0008. \tag{16}$$

This value compares well with previous estimates: Dean (1963), $p_c = 0.580 \pm 0.016$; Frisch *et al* (1961), $p_c = 0.573 \pm 0.017$; Sykes and Essam (1964b), $p_c = 0.590 \pm 0.010$.

We would like to mention in passing that it is possible, although a yeoman task, to count the complicated snakes for $N = 6$ using a computer to solve partial problems for different 'skeleton' snakes. This would be interesting in the light of equation (15) as one would then be able to focus p_c even further, not having to allow so wide a range for γ .

3. Size dependence of the singularity at p_c

The ideas discussed in the previous section, and the numerical work, allow certain insights into the nature of the singularity in the infinite system at $p = p_c$. The following discussion is for the percolation problem without snakes, ie without backward steps. The influence of the snakes would be, if any, to make the system more size dependent.

How sharp is the percolation threshold in a finite system? The uncertainty of the percolation density in the canonical ensemble (see appendix) as a function of N can be taken to be

$$\sigma_N \sim 1/P'_N(p_{cN}), \quad (17)$$

the inverse slope of $P_N(p)$ at the critical point. Writing $\sigma_N \sim N^{-\epsilon}$ we have

$$\epsilon = \lg P'_N(p_c)/\lg N \quad (18)$$

which we expect to approach a limit when $N \rightarrow \infty$. Numerically this seems to be so. With the use of (18) we obtain $\epsilon \simeq 0.67$.

We also looked, although somewhat indirectly, at the size effects in the microcanonical ensemble. We plotted the height of the peak of the function $N^2(\mu_n^{(N)} - \mu_{n-1}^{(N)})$ as a function of N and obtained the exponent $\tilde{\epsilon} = 0.49$, which suggests that the uncertainty of percolation in the microcanonical ensemble in terms of the variable n/N^2 behaves like

$$\sigma_\mu \sim N^{-0.49}.$$

In view of the analysis in the appendix this is slightly at odds with $\epsilon \simeq 0.67$ which should be equal to $\tilde{\epsilon}$ for large N .

Given that the snakes can only make the uncertainty even larger, the result for ϵ (or $\tilde{\epsilon}$) seems to us interesting. It says that percolation in finite systems is rather ill-defined. This may be of some importance in practical cases of percolation, particularly in biological systems where the number of units may be relatively small.

We would finally like to mention another aspect of the approach via finite systems. Through scaling arguments already referred to in connection with equation (3), or more easily with the following method also used by Imry and Bergman (1971), one can show that ϵ is directly related to a real critical exponent describing the divergence of the correlation length (average diameter of connected clusters below or disconnected lakes above p_{cN}) at p_{cN} . It is reasonable to assume that the correlation length in a finite system will have reached the linear size N of the system at $|p - p_{cN}| \sim 1/P'_N$. Assuming that the correlation length varies as $\xi \sim |p - p_{cN}|^{-\nu}$, we get from $\sigma_N \sim 1/P'_N \sim N^{-\epsilon}$:

$$\xi \sim N \sim |p - p_{cN}|^{-\nu} \sim N^{+\epsilon\nu}, \quad (19)$$

ie $\nu = 1/\epsilon$.

4. Numerical methods

The first step in the numerical analysis is to count, for given n and N , the number of percolating configurations. In the computer calculation it is natural to represent occupied sites by 1's and unoccupied sites by 0's. Each configuration can be represented by a string of N words each with N bits. Fast in-line logical comparison and bit-shifting functions can then be used to determine whether or not a given configuration percolates according to our rules.

By directly generating such strings and applying the percolation algorithm one can calculate the $k_n^{(N)}$ (see equation (5)) for $N \leq 5$. Since the number of configurations is 2^{N^2} , $N = 6$ already becomes very expensive however. A modification of the above method, in which the configurations are classified according to the percolation of substrings of the strings of N words, allowed the counting to proceed to $N = 9$ at modest cost (9 minutes on an IBM-370-165). A further investment was not considered worthwhile; extended results would improve estimates of the exponents somewhat, but would add little to our estimate of p_c because of the snake problem discussed above.

The second aspect of the numerical analysis is the extrapolation procedures for determining p_c and the exponents. Fortunately the sequence p_{cN} obtained from prescription (4) was quite convergent (as was the sequence \bar{p}_{cN}). Two extrapolation formulae were tried:

$$p_{cN} = p_{c\infty} + AN^{-\gamma} \quad (20a)$$

and

$$p_{cN} = p_{c\infty} + B e^{-\alpha N}. \quad (20b)$$

The free parameters p_c , A , γ or p_c , B , α were determined by fitting (20) to successive triplets of the p_{cN} . A sequence of values for the parameters, including p_c , results. If this sequence is reasonably constant then the assumed asymptotic form can be said to give a reasonable representation of the true asymptotic behaviour.

Typical results are shown in tables 2 and 3, which summarize fitting the form (20b) to the sequences \bar{p}_{cN} from equations (4) and (9). The last entry in the $\bar{p}_{c\infty}$ column gives a good estimate of the true $\bar{p}_{c\infty}$. This estimate can be further refined by extrapolating the sequence of $\bar{p}_{c\infty}$'s, although the numerical data may make this latter procedure either unnecessary or unwarranted.

The sequences p_{cN} and \bar{p}_{cN} from both equations (4) and (9) fitted the exponential form (20) significantly better than the power law form (20), and the sequences $1/\epsilon$ and $1/\bar{\epsilon}$

Table 2. Result of fitting the asymptotic form (20b) to successive triplets of \bar{p}_{cN} from equation (4).

N	$\bar{p}_{c\infty}$	B	α
1, 2, 3	0.475000	2.544	1.578
2, 3, 4	0.440931	0.907	0.926
3, 4, 5	0.429232	0.545	0.693
4, 5, 6	0.423662	0.375	0.562
5, 6, 7	0.421061	0.287	0.487
6, 7, 8	0.419816	0.236	0.441
7, 8, 9	0.419278	0.207	0.415

Table 3. Result of fitting the asymptotic form (20b) to successive triplets of \bar{p}_{cN} from equation (9).

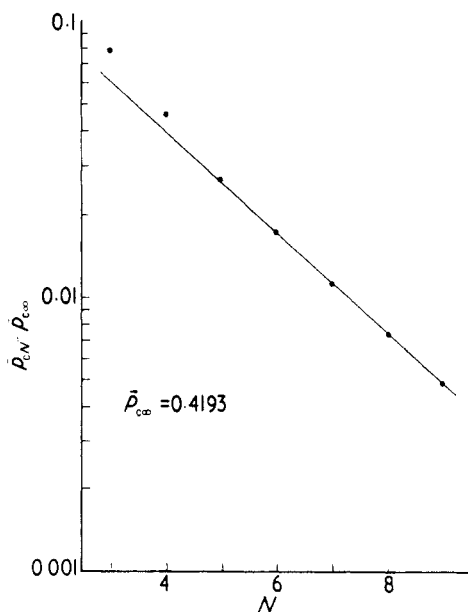
N	$\bar{p}_{c\infty}$	B	α
2, 3, 4	0.418058	0.1314	0.497
3, 4, 5	0.418714	0.1343	0.512
4, 5, 6	0.417473	0.1268	0.468
5, 6, 7	0.417022	0.1123	0.446
6, 7, 8	0.416922	0.1093	0.439
7, 8, 9	0.417022	0.1160	0.451

could not be fitted with the power law at all. The two sequences for \bar{p}_c (tables 2 and 3) seem to extrapolate to slightly different values of $\bar{p}_{c\infty}$. One would be inclined to take the extrapolated value from table 3, so stunningly good is the exponential fit, were it not that the last entry in the sequence for \bar{p}_c does not agree with the monotonically decreasing trend. A compromise between tables 2 and 3 is then indicated and we estimate $\bar{p}_{c\infty} = 0.4179 \pm 0.0014$, where the error limit contains both the last entry of table 2 on the high side and the result of the power law extrapolations to both sequences \bar{p}_{cN} on the low side. For $p_{c\infty}$ we quote $p_{c\infty} = 0.5907 \pm 0.0001$. The central value is from the fit to the last triplet ($N = 6, 7, 8$) of p_{cN} and the error limit contains both p_{c8} on the high side and the limit of the power law extrapolation on the low side.

In figure 6 $\bar{p}_{cN} - \bar{p}_{c\infty}$ from equation (4) are shown on a log plot as a function of N . If the data conform to (20) they should lie on a straight line.

The same procedure was applied to sequences $1/\epsilon$ and $1/\bar{\epsilon}$. The sequences of fits for $1/\epsilon$ and $1/\bar{\epsilon}$ were decreasing, appearing to lead to

$$1/\epsilon < 1.52 \quad (21a)$$

**Figure 6.** Log plot of $\bar{p}_{cN} - \bar{p}_{c\infty}$. The full curve is a straight line fit to the last three points.

and

$$1/\bar{\epsilon} < 1.53. \quad (21b)$$

No firm lower limits can be established from the numerical data, but the differences between successive fits for $1/\epsilon$ and $1/\bar{\epsilon}$ are quite small (less than 0.0004) and we would be surprised if $1/\epsilon$ or $1/\bar{\epsilon}$ were less than 1.50.

Note that if snakes did not exist one would have $1/\epsilon = 1/\bar{\epsilon}$. The sequence of fits for the exponents $\bar{\epsilon}$ and $\bar{\epsilon}$ were not monotonic because of irregularities induced by the truncation of the fractional part of $p_c N^2$. Parabolic interpolation smoothed the data considerably and we obtained an excellent fit for the height of the peak for $N \geq 4$.

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Appendix. Relation between 'microcanonical' and 'canonical' ensembles

The numerical data, the fractions of configurations $\mu_n = k_n / \binom{N^2}{n}$ with n filled sites that percolate, are in the microcanonical ensemble, n fixed. We calculate $P_N(p)$, the probability of percolation in the canonical ensemble, with the aid of the obvious transformation

$$P_N(p) = \sum_{n=0}^{N^2} \binom{N^2}{n} \mu_n p^n (1-p)^{N^2-n}. \quad (A.1)$$

The inverse transformation is complicated.

One can now determine p_c starting from the function $P_N(p)$ in the canonical ensemble as follows. One says that the distribution of densities at which different ensembles percolate is equal to $dP_N(p)/dp$. One then averages for the density at which percolation occurs (thus establishing equation (9)):

$$p_c = \int_0^1 \frac{dP_N(p)}{dp} p dp = \left| \int_0^1 P_N(p) p - \int_0^1 P_N(p) dp \right| = 1 - \frac{1}{N^2+1} \sum_{n=0}^{N^2} \mu_n. \quad (A.2)$$

The last step follows since the integral over p of any term in the binomial expansion of $[p+(1-p)]^M$ is equal to $(M+1)^{-1}$.

Another interesting question concerns the finite size effects in the different ensembles. Using (A.1) one can determine the width of the size-dependent region in the canonical ensemble, ie in the variable p , if the size-dependent region in n for the μ_n is given. We are interested in the width of the distribution $dP_N(p)/dp$. Starting with (A.1) at large N , replacing the sum over n with an integral over x and differentiating and integrating

$\mu(x) = \mu_n$ once with respect to x ,

$$\begin{aligned} \frac{dP_N(p)}{dp} &\simeq \frac{1}{p(1-p)} \int_0^{N^2} dz \int_0^z \frac{d\mu(x)}{dx} dx \frac{\Gamma(N^2+1)}{\Gamma(z+1)\Gamma(N^2-z+1)} p^z(1-p)^{N^2-z}(z-N^2p) \\ &= -\frac{1}{p(1-p)} \int_0^{N^2} dz \frac{d\mu(z)}{dz} \int_0^z \frac{\Gamma(N^2+1)}{\Gamma(x+1)\Gamma(N^2-x+1)} p^x(1-p)^{N^2-x}(x-N^2p) dx. \end{aligned} \tag{A.3}$$

The integrated term in the partial integration vanishes because the inner integral in the last form vanishes for $z = N^2$, as we will see shortly. For large N the function

$$f(x) = \frac{\Gamma(N^2+1)}{\Gamma(x+1)\Gamma(N^2-x+1)} p^x(1-p)^{N^2-x} \tag{A.4}$$

becomes a narrow Gaussian peak centred at pN^2 with $\sigma_p = N\sqrt{p(1-p)}$. ‘Narrow’ is to be understood on the scale of N^2 . We can then substitute the Gaussian in (A.3) and we realize that the integrand in the inner integral is essentially the derivative of the Gaussian peak with respect to x (and will vanish if integrated over the whole range of x as claimed above). We then have

$$\frac{dP_N(p)}{dp} = \int_0^{N^2} dz \frac{d\mu(z)}{dz} \frac{N^2}{[2\pi p(1-p)N^2]^{1/2}} \exp[-(z-N^2p)^2/2p(1-p)N^2]. \tag{A.5}$$

If now $d\mu/dz$, which also is a narrow peaked function on the scale of N^2 , varies slowly on the scale of σ_p the integral in (A.5) gives for $p = p_c$:

$$\left. \frac{dP_N(p)}{dp} \right|_{p_c} \simeq N^2 \left. \frac{d\mu(z)}{dz} \right|_{z=p_c N^2} \tag{A.6}$$

If, however, at the critical number of occupied sites, $d\mu/dz$ is a rapidly varying function, then

$$\left. \frac{dP_N(p)}{dp} \right|_{p_c} \simeq \frac{N^2}{[2\pi p_c(1-p_c)N^2]^{1/2}}. \tag{A.7}$$

Then (A.6) gives (σ_N defined in § 3)

$$\frac{1}{\sigma_N} \simeq N^2 \left. \frac{d\mu(z)}{dz} \right|_{z=p_c N^2} \simeq \frac{1}{\sigma_\mu}. \tag{A.8}$$

The factor N^2 in equation (A.8) changes the scale so that σ_μ is the uncertainty of percolation in the microcanonical ensemble in terms of the variable n/N^2 . On the other hand, equation (A.7) gives

$$\sigma_N \propto N^{-1}. \tag{A.9}$$

The conclusion is that as long as σ_μ vanishes more slowly than N^{-1} , σ_N and σ_μ will vary identically for large N . If, on the other hand, σ_μ vanishes more rapidly than N^{-1} , σ_N reflects the uncertainty in the number of occupied sites in the canonical ensemble rather than the uncertainty of percolation and varies as N^{-1} . The latter case could result from supplementary conditions on the occupation of the lattice such as an exclusion of too large fluctuations in the local density. This kind of condition would reduce the uncertainty in percolation stemming from adverse configurations.

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