LETTER TO THE EDITOR

Fluctuations in the number of percolation clusters*

A Coniglio†§, H E Stanley† and D Stauffer‡

†Center for Polymer Studies and Physics Department, Boston University, Boston, MA 02215, USA
‡Physics Department, University of Köln, Köln, West Germany

Abstract. For any lattice in any dimension the mean square fluctuation $\langle N_s^2 \rangle - \langle N_s \rangle^2$ in the numbers N_s of percolation clusters with s sites each is found to equal $\langle N_s \rangle$ for large clusters.

Although much accurate numerical information has been obtained recently on the average numbers $\langle N_s \rangle$ of clusters in the random percolation problem (Stoll and Domb 1978, Leath and Reich 1978, Nakanishi and Stanley 1978, Hoshen *et al* 1979), little is known so far about *fluctuations* in these (site) percolation quantities (Levinshtein *et al* 1976, Wu 1978). For example, if a large lattice is simulated many times on a computer, then in one realisation we may find ten clusters containing 100 sites each, in the next computer run we may find eight such clusters with $s = 100$ sites, and in the third simulation we may find twelve 100-clusters, etc. The average number $\langle N_s \rangle$ of such s-clusters is ten, and the mean square fluctuation of N_s is 8/3 in this example. How, in general, are these fluctuations $\langle N_s^2 \rangle - \langle N_s \rangle^2$ related to the averages $\langle N_s \rangle$? In particular, do these clusters behave like molecules in an ideal gas (if one cm³ contains 10^{20} molecules, the average fluctuation in this number is 10^{10} molecules cm⁻³), or do they show 'critical opalescence' (fluctuations are enhanced by a factor diverging at the critical point as the compressibility)? To answer this question, we calculate upper and lower bounds for these fluctuations (equation (8c)). For large cluster sizes s, the two bounds are found to coincide (equation (9)), and the final result is then tested and confirmed by Monte Carlo simulations (figure 1).

Let an s-cluster be a group of s occupied sites, connected by nearest-neighbour distances on a very large periodic lattice with N sites and coordination number z, in a random-site percolation problem for arbitrary dimensionality d, $1 \leqslant d < \infty$. The number of s-clusters in some realisation is N_s, whereas $P_s = \langle N_s \rangle s / N$ is the probability for an arbitrary lattice site to be part of an s-cluster, if each lattice site i, $i = 1, 2, \ldots, N$, is occupied randomly with probability p and is empty with probability $1 - p$. We denote by gamma symbols various characteristic functions which for each realisation are either unity or zero. In particular, if the superscript α denotes some s-cluster, then $\gamma_i^{s\alpha} = 1$ if lattice site i belongs to that cluster α, and $\gamma_{ij}^{s\alpha} = 1$ if the two sites i and j belong to the same cluster α. Otherwise these characteristic functions are zero. Consequently, $\gamma_i^s \equiv \Sigma_\alpha \gamma_i^{s\alpha}$ equals unity if site i belongs to any s-cluster, and $\gamma_{ij}^s \equiv \Sigma_\alpha \gamma_{ij}^{s\alpha}$ equals unity if both i and j belong to the same s-cluster—otherwise these sums vanish, since by
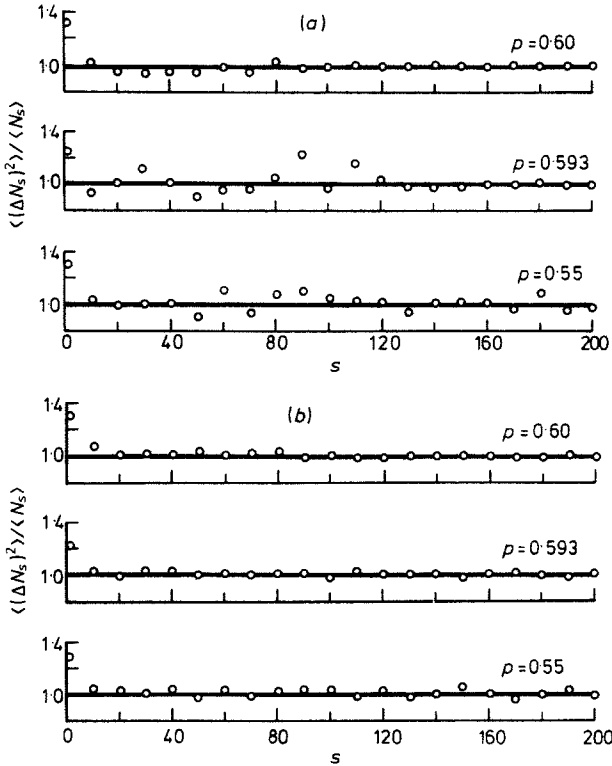
Figure 1. (a) Relative fluctuation $(\langle N_s^2 \rangle - \langle N_s \rangle^2)/\langle N_s \rangle$ in the cluster numbers, for 1000 runs on a 100×100 square lattice, as a function of s for three different values of p. To improve the statistics, in (b) the fluctuations have been averaged over the ten previous s values. Asymptotically the Monte Carlo points tend to unity according to prediction (9).

definition no sites belong to two different clusters α and α' in any given configuration. If we average these characteristic functions over many realisations of the same lattice on a computer, we find the probabilities $P_s = \langle \gamma_i^s \rangle$ and $P_{ij}^s = \langle \gamma_{ij}^s \rangle$, where P_{ij}^s is the probability for the sites i and j to belong to the same s-cluster, and is connected with the density profile of s-clusters. In a large lattice nearly all sites i are equivalent, and we can rewrite these results in the thermodynamic limit as

$$\left\langle \sum_i \gamma_i^s \right\rangle = NP_s = s\langle N_s \rangle, \tag{1a}$$

$$\left\langle \sum_{ij} \gamma_{ij}^s \right\rangle = sNP_s = s^2 \langle N_s \rangle. \tag{1b}$$

If we define

$$\Delta_{ij}^s \equiv \langle \gamma_i^s \gamma_j^s \rangle - \langle \gamma_i^s \rangle \langle \gamma_j^s \rangle \tag{1c}$$

as a 'density–density' correlation function due to s-clusters (note that $\gamma_i^s \gamma_j^s = 1$ if i and j belong to two different s-clusters), then we have, from equation (1a),

$$\sum_{ij} \Delta_{ij}^s = s^2 (\langle N_s^2 \rangle - \langle N_s \rangle^2). \tag{1d}$$

This is the quantity we are interested in.

We now express Δ_{ij}^s in a different way, noting that for a given configuration two s-clusters α and α' are either identical or do not overlap at all. In the second case, either they have some common perimeter sites ('touching') or these perimeters do not overlap ('separated'). (The 'perimeter' sites are empty sites which have occupied cluster sites as neighbours.) By α'_n we denote a cluster α' which has n perimeter sites in common with cluster α; thus α'_0 denotes a cluster separated from the cluster α. This distinction between identical, touching, and separated pairs α and α' of clusters gives

$$\langle \gamma_i^s \gamma_j^s \rangle = \sum_{\alpha\alpha'} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'} \rangle = P_{ij}^s + \sum_{\alpha\alpha'_0} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_0} \rangle + \sum_{\alpha\alpha'_n} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle. \tag{2a}$$

For separate clusters we have statistical independence,

$$\langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_0} \rangle = \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_0} \rangle, \tag{2b}$$

whereas

$$\langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle = (1-p)^{-n} \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_n} \rangle \tag{2c}$$

for touching clusters.

Similarly,

$$\langle \gamma_i^s \rangle \langle \gamma_j^s \rangle = \sum_{\alpha\alpha'} \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle = {\sum_{\alpha\alpha'}}' \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle + \sum_{\alpha\alpha'_0} \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_0} \rangle + \sum_{\alpha\alpha'_n} \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_n} \rangle, \tag{3}$$

where the prime on the first sum indicates summation over those cluster pairs which have at least one cluster site in common. (Note that in such a case for $\alpha \neq \alpha'$ we have $\gamma_i^{s\alpha} \gamma_j^{s\alpha'} = 0$ for every configuration, but $\langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle \neq 0$ since these different averages involve different realisations.) Combining equations $(1c)$, (2) and (3), we find that the separated clusters cancel out:

$$\Delta_{ij}^s = P_{ij}^s - {\sum_{\alpha\alpha'}}' \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle + \sum_{\alpha\alpha'_n} (\langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle - \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_n} \rangle). \tag{4}$$

To find upper and lower bounds for Δ_{ij}^s and thus, by equation $(1d)$, for the fluctuations in the cluster numbers N_s, we need two inequalities:

$$\sum_k P_{ik}^s P_{kj}^s \geq {\sum_{\alpha\alpha'}}' \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle \tag{5}$$

and

$$(2s+1)^{-1} p(1-p)^{z-3} \sum_{\alpha\alpha'_n} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle \leq P_{ij}^{2s+1}. \tag{6}$$

Proof. Every pair (α, α') in the RHS of equation (5) has by definition (note the prime!) at least one common cluster site k, and for this k we have $\langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'} \rangle = \langle \gamma_{ik}^{s\alpha} \rangle \langle \gamma_{jk}^{s\alpha'} \rangle$. The LHS of equation (5) equals

$$\sum_{\alpha\alpha'} \sum_k \langle \gamma_{ik}^{s\alpha} \rangle \langle \gamma_{jk}^{s\alpha'} \rangle,$$

since $P_{ik}^s = \sum_\alpha \langle \gamma_{ik}^{s\alpha} \rangle$. Therefore every term in the RHS of equation (5) is contained in the sum on the LHS of equation (5), which proves inequality (5).

Equation (6) is more difficult to prove. From every pair (α, α'_n) of touching s-clusters on the LHS of equation (6), we can construct a single cluster, called α'', with $2s+1$ sites, by filling one of the n common perimeter sites of the two clusters α and α'. The cluster probabilities are then connected by

$$\langle \gamma_{ij}^{2s+1,\alpha''} \rangle = a \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle,$$

where the constant a contains the factors arising from the creation of one new cluster site (factor p), the filling of one perimeter site (factor $1/(1-p)$), and the possible creation of new perimeter sites (factor $1-p$ for each). Since at most $z-2$ new perimeter sites are created in a lattice with coordination number z, we have $p(1-p)^{-1} \geq a \geq p(1-p)^{z-3}$, or $\langle \gamma^{2s+1,\alpha''} \rangle \geq p(1-p)^{z-3} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle$. Consequently, $p(1-p)^{z-3} \Sigma_{\alpha\alpha'_n} \langle \gamma_i^{s\alpha} \gamma_j^{s\alpha'_n} \rangle \leq (2s+1)\Sigma_{\alpha''} \langle \gamma_{ij}^{2s+1,\alpha''} \rangle$ which proves inequality (6) (the factor $2s+1$ arises from the fact that at most $2s+1$ different pairs (α, α'_n) give the same α''). This completes our derivation of equations (5) and (6).

Combining inequality (5) with equations (2c) and (4), we obtain

$$\Delta_{ij}^s \geq P_{ij}^s - \sum_k P_{ik}^s P_{kj}^s, \tag{7a}$$

by omitting touching clusters in equation (4). On the other hand, from inequality (6) we find, by omitting the overlapping clusters in equation (4),

$$\Delta_{ij}^s \leq P_{ij}^s + b_s P_{ij}^{2s+1} - \sum_{\alpha\alpha'_n} \langle \gamma_i^{s\alpha} \rangle \langle \gamma_j^{s\alpha'_n} \rangle \leq P_{ij}^s + b_s P_{ij}^{2s+1}, \tag{7b}$$

with $b_s = (2s+1)(1-p)^{3-z}/p \gg 1$. Thus equations (7a) and (7b) give the desired upper and lower bounds for Δ_{ij}^s.

Now we sum equations (7a) and (7b) over the two lattice sites i and j, where $\Sigma_{ij} P_{ij}^s = s^2 \langle N_s \rangle$ from equation (1b) and $\Sigma_{ijk} P_{ik}^s P_{kj}^s = N^{-1}(\Sigma_{ik} P_{ik}^s)(\Sigma_{km} P_{km}^s) = (s^2 \langle N_s \rangle)^2 / N$. Thus

$$\sum_{ij} \Delta_{ij}^s \geq s^2 \langle N_s \rangle - (1/N)s^4 \langle N_s \rangle^2 \tag{8a}$$

and

$$\sum_{ij} \Delta_{ij}^s \leq s^2 \langle N_s \rangle + b_s(2s+1)^2 \langle N_{2s+1} \rangle \tag{8b}$$

from equations (7). These results give, with equation (1d), the desired upper and lower bounds for the fluctuations:

$$1 - s^2 \langle N_s \rangle / N \leq (\langle N_s^2 \rangle - \langle N_s \rangle^2)/\langle N_s \rangle \leq 1 + b_s(2+1/s)^2 \langle N_{2s+1} \rangle / \langle N_s \rangle. \tag{8c}$$

This inequality is our main exact result. As they should be, the mean square fluctuations $\langle N_s^2 \rangle - \langle N_s \rangle^2$ are proportional to the size N of the system, as are the averages $\langle N_s \rangle$.

For large enough s we know (Stoll and Domb 1978, Leath and Reich 1978, Hoshen *et al* 1979) that the cluster numbers $\langle N_s \rangle$ decay rapidly (exponentially) with increasing cluster size s, except at $p = p_c$. Thus for $s \to \infty$ at fixed p (and fixed lattice size N) we have $s^2 \langle N_s \rangle \to 0$, and for $p \neq p_c$ we also have $b_s \langle N_{2s+1} \rangle / \langle N_s \rangle \to 0$; therefore the upper and lower bounds coincide for large clusters in equation (8c):

$$(\langle N_s^2 \rangle - \langle N_s \rangle^2)/\langle N_s \rangle \to 1 \qquad (s \to \infty, p \neq p_c). \tag{9}$$

Our Monte Carlo tests of prediction (9) are presented in figure 1, using the Hoshen methods employed by Nakanishi and Stanley (1978) to generate and count percolation clusters. Our computer studies confirm that the ratios $(\langle N_s^2 \rangle - \langle N_s \rangle^2)/\langle N_s \rangle$ are close to unity, even at p_c where our inequalities are somewhat inconclusive. Thus

$$\langle N_s^2 \rangle - \langle N_s \rangle^2 \approx N_s \tag{10}$$

is a good approximation even for rather small clusters, both away from p_c and at p_c, and equation (10) thus gives a simple estimate of Monte Carlo errors in cluster counts.

Finally, we return to our initial question: do the clusters behave like molecules in an ideal gas, or do they show critical opalescence in the cluster numbers? Our answer is both yes and no. Our final result, (10), looks just like the fluctuations in the number of molecules per cm^3 for an ideal gas, without an enhancement factor due to interactions. But, in contrast to the ideal gas case, our average numbers N_s are not fixed but have, for large s as a function of p, a very sharp peak very close to the critical concentration p_c, whereas they are extremely small away from p_c. In this sense the $\langle N_s \rangle$, and thus also the fluctuations $\langle N_s^2 \rangle - \langle N_s \rangle^2$, show a strong critical opalescence. Thus, although the statistical error can be estimated very easily by the usual square root law of ideal systems, equation (10), that same equation also shows the strong critical opalescence in the fluctuations characteristic of cooperative phenomena.

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