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Series expansions in a continuum percolation problem†

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Abstract. Power series in number density are used to study the distribution of cluster sizes in a continuum analogue of bond percolation on a lattice. The clusters are formed by overlapping of geometrical regions that are randomly distributed in space. The regions are circles and oriented squares in two dimensions, and spheres and oriented cubes in three dimensions. The power series are based on a graphical expansion, using topological weights from percolation theory and probabilities obtained from cluster integrals. Analysis of the mean cluster size series provides estimates of the critical percolation density, and the associated critical exponent. The critical densities are consistent with previous Monte Carlo evaluations, and the exponents are close to those found for the corresponding lattice problems.

1. Introduction

In this paper, series expansion techniques are used to discuss certain critical properties of a continuum analogue of bond percolation on a lattice. The problem is defined as follows. N points are randomly distributed in a volume Ω. A geometrical region (e.g. a sphere) is centred on each point. If two such regions overlap, their centres are said to be connected, and to form part of a cluster. In this way, any given configuration of points is associated with a set of clusters of various sizes. This is illustrated in figure 1, where nine points are divided into two clusters of size one (isolated points), two clusters of size two, and one cluster of size three. As in lattice percolation theory, one wishes to know the distribution of cluster sizes in the limit where N and Ω are very large, and their ratio $\rho = N/\Omega$ is fixed. This is obtained by averaging over all random configurations of points having density ρ. In particular, one would like to know the critical density ρ_c at which macroscopically large clusters first appear. Also, one would like to determine critical exponents associated with the behaviour of the cluster size distribution near the critical density.

The continuum percolation problem arises in several models for physical systems (Holcomb and Rehr 1969, Pike and Seager 1974). It has been studied by numerical simulation (most recently, Fremlin 1976), and also as a limit of certain lattice percolation problems (Domb 1972).

We have evaluated a number of terms in the power series expansion, in density, of the mean number of clusters of a given size, the mean number of clusters of any size, and the mean cluster size. The geometrical regions defining 'overlap' are taken to be circles

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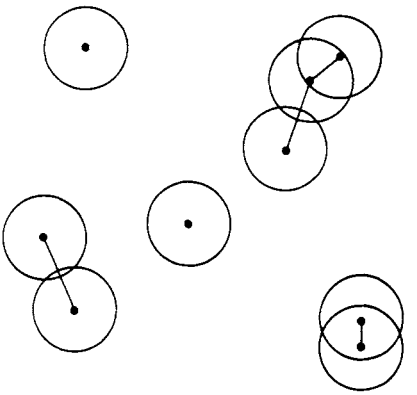

Figure 1. Division of a configuration into clusters.

or oriented squares in two dimensions, and spheres or oriented cubes in three dimensions.

A ratio analysis of the series coefficients for mean cluster size, for the four cases just listed, provides numerical estimates for the corresponding critical percolation densities. Our results agree resonably well with previous estimates. The ratio analysis also provides estimates for the critical exponent γ determining the divergence of the mean cluster size at ρ_c. In accordance with a conjecture of Sykes and Essam (1964), that the critical exponents are dimensional invariants, our values of γ are consistent with those found for lattice percolation. Our results also compare favourably with one numerical simulation (Roberts 1967) which produced 'experimental data' on the mean cluster size for circles as a function of density.

2. Derivation of series

For a configuration of N points, the continuum percolation problem is similar to bond percolation on the complete graph K_N (we follow the terminology of Essam and Fisher 1970). (No analogy is perfect. In some respects, the problem dealt with here is also an analogue of site percolation. In developing the basic equation (2.6), we found it useful to focus on the analogy to bond percolation; at equation (2.9), an analogy to site percolation is evident. The results are, of course, not affected by the point of view taken in obtaining them.) In bond percolation on a lattice, a fraction p of the edges of a lattice, randomly chosen, are designated as 'coloured'; clusters are defined as subgraphs of vertices connected by strings of coloured edges. In the continuum problem, the lattice is replaced by the complete graph K_N, and 'coloured' is replaced by 'overlapping'. In both cases one requires certain topological *weights*, associated with the subgraphs which can be embedded in the lattice or in K_N. However, the *probabilities* associated with these subgraphs are different. In bond percolation on a lattice, the probability of a subgraph G having $e(G)$ edges is $p^{e(G)}$; in the continuum problem, the probability is obtained from a cluster integral which measures the volume of configuration space available for that subgraph.

To show the similarities and differences, it is convenient to use a notation which includes both continuum and lattice bond percolation. Let K be the graph on which

calculations are to be performed; this is either the lattice L or the complete graph K_N. Let $\boldsymbol{R}$ denote a particular configuration; this is either the set of coloured edges, or the positions of N points in a volume Ω. We associate a characteristic function with each edge $\alpha = [i, j]$ of the graph K:

$$\begin{aligned} &\text{lattice} \qquad f_{[i,j]}(\boldsymbol{R}) = \begin{cases} 1 & \text{if } [i,j] \text{ is coloured} \\ 0 & \text{otherwise,} \end{cases} \\ &\text{continuum} \qquad f_{[i,j]}(\boldsymbol{R}) = \begin{cases} 1 & \text{if regions } i \text{ and } j \text{ overlap} \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{2.1}$$

A cluster in the configuration $\boldsymbol{R}$ corresponds to a connected subgraph H of K in the obvious way: the vertex set $V(H)$ is the set of points in the cluster, and the edge set $E(H)$ is the set of coloured or overlap bonds in the cluster. Then a given subgraph $H \subseteq K$ has a characteristic function which is unity if H is truly a cluster in $\boldsymbol{R}$, and zero otherwise,

$$F(H; \boldsymbol{R}, K) = \prod_{\alpha \in E(H)} f_\alpha(\boldsymbol{R}) \cdot \prod_{\beta \in E_K(H)} (1 - f_\beta(\boldsymbol{R})). \tag{2.2}$$

Here, $E_K(H)$ is the edge perimeter of H in K, i.e. those edges which if coloured would make the cluster larger or introduce new edges within H. The number of clusters of size s is found by summing the characteristic function over all connected subgraphs of K which have s vertices,

$$n_s(\boldsymbol{R}, K) = \sum_{\substack{c \\ H \subseteq K \\ V(H) = s}} F(H; \boldsymbol{R}, K). \tag{2.3}$$

By expanding the product $\Pi(1 - f_\beta)$ and re-ordering the summations in the resulting expression for n_s, we obtain

$$n_s(\boldsymbol{R}, K) = \sum_{G \subseteq K}{}_c \, w_s(G) \prod_{\alpha \in E(G)} f_\alpha(\boldsymbol{R}). \tag{2.4}$$

The weights $w_s(G)$ are given by

$$w_s(G) = (-1)^{e(G)} \sum_{H \subseteq G}{}' (-1)^{e(H)}, \tag{2.5}$$

where $e(G)$ is the number of edges in G, and the primed sum is over all $H \subseteq G$ which are connected, have s vertices, and have full edge perimeter in G (i.e. any edge of G not in H is adjacent to a vertex of H). Note that $w_s(G)$ is independent of the starting graph K. The average number of clusters of size s is found by averaging (2.4) over all configurations. We are concerned here with the average number of clusters per point in the thermodynamic limit, or

$$\langle n_s; K \rangle = N^{-1} \sum_{G \subseteq K}{}_c \, w_s(G) \left\langle \prod_{\alpha \in E(G)} f_\alpha(\boldsymbol{R}) \right\rangle. \tag{2.6}$$

From here on, the lattice and continuum problems must be treated differently.

First, we consider the lattice problem. The number of embeddings of a free connected graph c in L is proportional to N as N goes to infinity. There is no correlation between probabilities that distinct edges are coloured, so the average in

(2.6) may be factored. The average of a single f_α is just p, the fraction of coloured bonds. Then (2.6) becomes

$$\langle n_s; L\rangle = \sum_c (c; L) N^{-1} w_s(c) p^{e(c)} \tag{2.7}$$

where $(c; L)N^{-1}$ is the number of embeddings, per site, of c in L. This result, an explicit power series in p, is familiar in lattice percolation theory.

In the continuum problem, the averages in (2.6) are related to cluster integrals. We define a quantity which remains finite, for a connected graph, in the limit of infinite volume Ω,

$$I(G) = \Omega^{-1} \int \mathrm{d}R^{V(G)} \prod_{\alpha \in E(G)} f_\alpha. \tag{2.8}$$

The integral is taken over the positions of the points in the vertex set of G. It has exactly the same structure as the cluster integrals that occur in the virial theory of the equation of state of a hard sphere gas (or a hard cube gas, etc). As long as we are concerned only with clusters such that $V(c) \ll N$, (2.6) becomes

$$\langle n_s\rangle = \sum_c (\rho^{V(c)-1}/V(c)!)(c; K_{V(c)}) w_s(c) I(c). \tag{2.9}$$

where $(c; K_{V(c)})$ is the number of ways to label c. This is the final form, to be compared with (2.7).

3. Results and analysis

To complete the calculation of the cluster size distribution, we need the weights $w_s(c)$, the integrals $I(c)$, and the cominatorial factors $(c; K_{V(c)})$. The weights are those used in bond percolation theory. This means that they have already been determined for small graphs which can be embedded in common lattices. In the continuum problem, however, we need them also for graphs which can be embedded in K_N but not in lattices. We calculated these ourselves, using techniques put forth by Essam (1972).

The integrals and the combinatorial factors arise in the virial theory of the equation of state of a gas, and considerable information is available. The integrals have been evaluated up to five point graphs for spheres (Kilpatrick 1971) and for circles (Kratky 1976), and up to seven point graphs for oriented squares and cubes (Hoover and DeRocco 1962). Some information is available for six point graphs for circles and spheres (Ree and Hoover 1964); we shall return to this shortly.

The mean number of clusters, and the mean cluster size, are obtained from (2.9) by summing over s, with weights 1 and s^2. In the series for the mean number of clusters, the resulting weights are the weak K-weights; these vanish for reducible graphs. The mean cluster size expansion requires all connected graphs; but in the continuum problem, contributions from reducible graphs can be summed directly, so that only irreducible graphs are needed. This formal summation of reducible graphs is described in the appendix.

Our calculations were limited by the availability of the integrals $I(c)$. With two exceptions, we went as far as possible with this limitation. In one case, the mean number of clusters, we were able to get a fifth order term for circles by using a different

form of (2.9). It is possible to rewrite the series in terms of different integrals $J(G)$,

$$J(G)=\Omega^{-1}\int \mathrm{d}R^{V(G)} \prod_{\alpha\in E(G)} f_\alpha \prod_{\beta\in E(\bar{G})}(1-f_\beta), \tag{3.1}$$

where $\bar{G}$ is the complementary graph of G. The weights in this form of the expansion are the strong weights of percolation theory. Because the virial expansion can also be transformed to a series involving the $J(G)$ integrals (Ree and Hoover 1964), some of these have been calculated for circles and spheres. Unfortunately for our purposes, many irreducible graphs have zero weight in this form of the virial expansion, and consequently the integrals for these graphs were not evaluated. In the case of circles, one six point graph has zero weight in the virial expansion and non-zero strong K-weight in the mean number expansion. However, $J(G)$ is known to vanish for this particular graph, so that we were able to complete the mean number expansion for circles to the fifth order term.

Table 1. Numerical results. All series are in $b = 1$ units (see (3.1) in text). The numbers in parentheses are error estimates according to the standard convention; all other numbers are accurate to the digits listed. In all cases $\langle n_1\rangle$ is $e^{-2\rho}$.

	ρ^0	ρ^1	ρ^2	ρ^3	ρ^4	ρ^5	ρ^6
Circles							
$\langle n_2\rangle$		1	−2·8270	4·0364	−3·8776		
$\langle n_3\rangle$			1·2180	−4·4168	8·11055		
$\langle n_4\rangle$				1·6277	−7·1764		
$\langle n_5\rangle$					2·2955		
$S(\rho)$	1	2	1·6540	1·1045	0·67129		
$K(\rho)$	1	−1	0·39100	−0·085968	0·013706	$-1\cdot59(4)\times10^{-3}$	
Squares							
$\langle n_2\rangle$		1	−2·87500	4·18056	−4·09590	3·03934	
$\langle n_3\rangle$			1·25000	−4·63889	8·72222	−11·0685	
$\langle n_4\rangle$				1·72222	−7·79299	17·8672	
$\langle n_5\rangle$					2·50608	−13·3485	
$\langle n_6\rangle$						3·77788	
$S(\rho)$	1	2	1·750000	1·194444	0·7473958	0·4404861	0·2494164
$K(\rho)$	1	−1	0·3750000	−0·06944444	$6\cdot076388\times10^{-3}$	$7\cdot118056\times10^{-4}$	$3\cdot590375\times10^{-4}$
Spheres							
$\langle n_2\rangle$		1	−3·0625	4·7222	−4·8848		
$\langle n_3\rangle$			1·3750	−5·6159	11·5591		
$\langle n_4\rangle$				2·1842	−11·1039(1)		
$\langle n_5\rangle$					3·7683(1)		
$S(\rho)$	1	2	2·1250	1·9588	1·703(2)		
$K(\rho)$	1	−1	0·31250	−0·042862	$5\cdot31(2)\times10^{-3}$		
Cubes							
$\langle n_2\rangle$		1	−3·15625	5·02200	−5·36730	4·33207	
$\langle n_3\rangle$			1·43750	−6·11343	13·1156	−18·9149	
$\langle n_4\rangle$				2·40741	−12·8069	34·3619	
$\langle n_5\rangle$					4·38979	−27·9653	
$\langle n_6\rangle$						8·45436	
$S(\rho)$	1	2	2·312500	2·252315	2·071425	1·838835	1·596086
$K(\rho)$	1	−1	0·2812500	−0·01736111	$-2\cdot040473\times10^{-3}$	$1\cdot576968\times10^{-3}$	$-3\cdot684968\times10^{-5}$

Also, because of the large number of connected seven point graphs, we evaluated the sixth order terms only for those series that could be obtained from irreducible graphs, i.e. the mean cluster number and the mean cluster size.

The numerical results of these calculations are presented in table 1. The series are all expressed in terms of a density variable $b\rho$ chosen to make the leading terms identical in each case. The quantity b is defined as in the virial expansion,

$$b = \tfrac{1}{2}I(K_2) \tag{3.2}$$

$$b = \begin{cases} \frac{1}{2}\pi\sigma^2 & \text{(circles)} \\ 2\sigma^2 & \text{(squares)} \\ \frac{2}{3}\pi\sigma^3 & \text{(spheres)} \\ 4\sigma^3 & \text{(cubes).} \end{cases} \tag{3.3}$$

Note that $2b$ is the volume surrounding each point in which another point would be 'connected' to the first one.

The critical density ρ_c and the critical exponent γ of the mean cluster size $S(\rho)$ were estimated by conventional ratio analysis of the series, based on an assumed asymptotic form $(\rho_c - \rho)^{-\gamma}$. Figure 2 shows how the ratios a_n/a_{n-1} behave as a function of $1/n$ for cubes; from this graph one can get a rough estimate of ρ_c and γ. We used a variety of methods to sharpen our results—graphical analysis, Neville tables, and Padé approximants. The series are rather short, and there is considerable spread in the results. The numbers presented in table 2 are our best guesses. This table also presents results obtained by other investigators. The agreement is reasonable. In particular, the exponent γ for the continuum problem is, within our rather wide error bounds, identical with the corresponding exponent for bond percolation on a lattice.

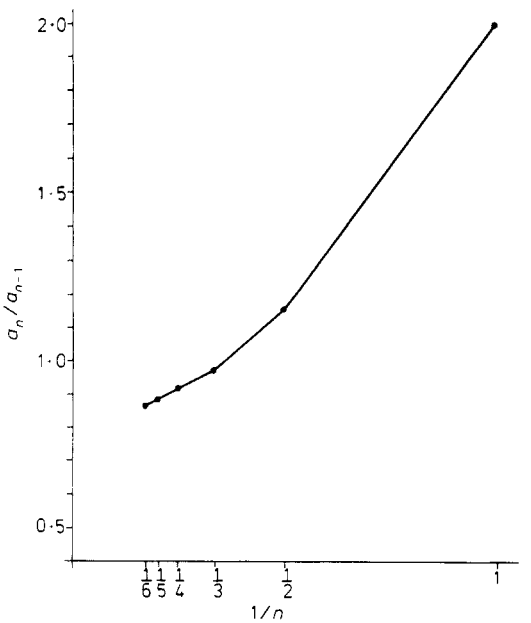

Figure 2. Ratios for cluster size expansions (cubes).

Table 2. Estimates of the critical density and the exponent for the mean cluster size. The lattice exponents are from Sykes *et al* (1976) and Sykes and Essam (1964).

	Spheres	Cubes	Circles	Squares
ρ_c (percolation density)				
New value	$1{\cdot}40 \pm 0{\cdot}1$	$1{\cdot}29 \pm 0{\cdot}02$	$2{\cdot}3 \pm 0{\cdot}15$	$2{\cdot}20 \pm 0{\cdot}02$
Pike and Seager (1974)	$1{\cdot}33 \pm 0{\cdot}05$†		$2{\cdot}25 \pm 0{\cdot}1$	$2{\cdot}23 \pm 0{\cdot}1$†
Gayda and Ottavi (1974)	$1{\cdot}33 \pm 0{\cdot}05$			
Ottavi and Gayda (1974)			$2{\cdot}05 \pm 0{\cdot}1$	
Kurkijarvi (1974)	$1{\cdot}38 \pm 0{\cdot}04$			
Roberts (1967)			$1{\cdot}91 \pm 0{\cdot}08$	
Holcomb *et al* (1972)	1·17			
Domb (1972)	$1{\cdot}36 \pm 0{\cdot}1$†		$2{\cdot}25 \pm 0{\cdot}25$†	
Fremlin (1976)	$1{\cdot}35 \pm 0{\cdot}05$		$2{\cdot}20 \pm 0{\cdot}1$	
γ (exponent for mean cluster size)				
New value	$1{\cdot}80 \pm 0{\cdot}2$	$1{\cdot}70 \pm 0{\cdot}1$	$2{\cdot}60 \pm 0{\cdot}2$	$2{\cdot}45 \pm 0{\cdot}1$
Lattice	$1{\cdot}69 \pm 0{\cdot}05$	$1{\cdot}69 \pm 0{\cdot}05$	$2{\cdot}43 \pm 0{\cdot}03$	$2{\cdot}43 \pm 0{\cdot}03$

† These are our error estimates based on the authors' discussions.

The reader should note that there are difficulties in applying standard ratio analyses to the mean cluster size series in lattice percolation. The radius of convergence in p is determined by weak singularities off the real p axis, and the series must be analysed with Padé approximants or similar techniques (Sykes *et al* 1973). However, low order terms on the series appear to be dominated by the physical singularity, and give proper estimates of ρ_c and γ. We hope that the same is true in our analysis.

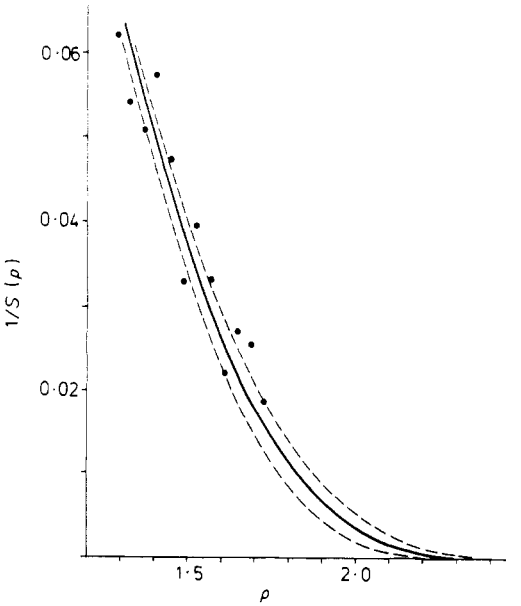

Figure 3. Comparison with Monte Carlo data (circles).

There has been considerable discussion in the literature of a discrepancy between the critical densities obtained by Roberts (1967) and by Holcomb *et al* (1972), and the critical densities obtained by other workers. The discrepant values are based on a scheme in which the mean cluster size is actually measured for random configurations generated by computer. These authors plot $1/S(\rho)$ against ρ and extrapolate linearly to $1/S(\rho_c)=0$. It is likely that the linear extrapolation yields an underestimate of ρ_c. We have tested this by providing our own theoretical fit to the computer data. For use in the circles case, the function

$$S(\rho)=16{\cdot}77(2{\cdot}3-\rho)^{-2{\cdot}43}-1{\cdot}22-0{\cdot}34\rho-0{\cdot}092\rho^2 \tag{3.4}$$

has the critical density $\rho_c=2{\cdot}3$, exponent $\gamma=2{\cdot}43$, and its series expansion agrees with ours to the fourth power of density. In figure 3, this function is compared with Roberts' experimental data. The broken curves show what happens when ρ_c is changed to 2·2 and to 2·4. The agreement with Roberts' data is about as good as can be expected. The linear extrapolation gives $\rho_c \cong 1{\cdot}9$.

Appendix. Summation of reducible graphs in cluster size expansion

The summation follows from results of Essam (1971). He denotes the weight for the mean cluster size expansion as m_{02}, so that the expansion we need is

$$S(\rho)=\sum_c \rho^{V(c)-1}\frac{1}{V(c)!}(c;K_{V(c)})m_{02}(c)I(c). \tag{A.1}$$

The weight m_{02} is related to another weight $d(G^{ii})$, called the pair connectedness weight of the two-rooted graph G^{ii}; the relation is

$$m_{02}(G)=2\sum_t d(G_t^{ii}), \tag{A.2}$$

where the sum is over all two-rootings of G. Essam shows that the only reducible two-rooted graphs with non-zero $d(G_t^{ii})$ are those with a string structure; that is, G is made up of n two-rooted irreducible subgraphs $H_1^{ii}, H_2^{ii}, \ldots, H_n^{ii}$, with $n \geqslant 0$, and two one-rooted irreducible subgraphs L_1^i and L_2^i, all joined at their roots to form a string $L_1^i H_1^{ii} H_2^{ii} \ldots H_n^{ii} L_2^i$. Furthermore, the only two-rootings of G with non-zero $d(G_t^{ii})$ are those with one root in L_1^i and one in L_2^i. So the sum over two-rootings in (A.2) becomes a sum over the ways to set additional roots t_1 in L_1^i and t_2 in L_2^i. For two-rootings of this form, $d(G_t^{ii})$ factors and we have

$$m_{02}(G)=2d(H_1^{ii})d(H_2^{ii})\ldots d(H_n^{ii})\sum_{t_1} d(L_{1t_1}^{ii})\sum_{t_2} d(L_{2t_2}^{ii}). \tag{A.3}$$

We also have that

$$I(G)=I(L_1^i)I(H_1^{ii})I(H_2^{ii})\ldots I(H_n^{ii})I(L_2^i). \tag{A.4}$$

The sum in (A.1) may now be separated into a sum over n and over the irreducible subgraphs. Note that each combination of subgraphs corresponds to 2^n string graphs G

because one must decide which root of H_j^{ii} attaches to H_{j+1}^{ii}. Performing the sum over n and using (A.2) to go back to the m_{02} weights, we obtain

$$S(\rho) = (1 - S_s(\rho))^{-1}. \tag{A.5}$$

Here $S_s(\rho)$ is the same as (A.1) except that the sum is only over stars.

The result holds only for the random configurations problem, and not for bond percolation on a lattice. The essential difference is that, in a lattice, the embedding of one part of a string graph constrains how the rest of it may be embedded; in a random configuration, there is no such interaction between the constituents of the string.

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