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Aspects of the structure of the infinite cluster in site percolation

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Abstract. In this paper we present the results of preliminary investigations into the structure of the infinite cluster in site percolation theory. It is shown how series expansions, for quantities defined as site and bond valency respectively, may be derived. The series are used to obtain a measure of the degree of ramification of the infinite cluster, and techniques for obtaining a free energy series for the infinite cluster in a site-dilute ferromagnet are discussed.

1. Introduction

The investigation in this paper relates to the nature of the infinite cluster in site percolation for the simple quadratic, triangular and simple cubic lattices. We shall consider the problem in terms of magnetic and non-magnetic sites, distributed with probabilities p and q, respectively, such that $p+q=1$. Quantities termed site valency and bond valency are obtained in the form of series expansions for the infinite cluster (IC). The former is denoted by $D^{\mathrm{I}}(v, q)$ and represents the probability of a site in the IC having valency v (i.e. having v adjacent magnetic sites). The latter is denoted by $B^{\mathrm{I}}(l, m, q)$ and represents the probability of a bond in the IC having sites of valency l and m at either end.

It is then shown how these series may be used to obtain estimates for lambda, a quantity defined originally by Domb and Stoll (1977) as a measure of the degree of ramification of the IC.. The highly ramified nature just above the percolation threshold is demonstrated, and the steady increase in compactness as q decreases to zero. Finally techniques are introduced by which we hope in the future to derive low-temperature expansions for the free energy of the IC.

2. Site valency for the entire system

When we consider the entire system, i.e. that composed of both finite and, if present, infinite clusters, we may define a quantity $D^{\mathrm{E}}(v, q)$ which denotes the probability of a site in the entire system having valency v. Clearly we then have

$$D^{\mathrm{I}}(v, q)=\frac{D^{\mathrm{E}}(v, q)-\Sigma_i D_i^{\mathrm{F}}(v, q)}{(1-q)} \tag{2.1}$$

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in which $D_i^F(v, q)$ is simply the probability of a site being in the ith cluster of finite size and having valency v. The summation runs over all finite clusters, and the factor $(1-q)$ in the denominator arises from the fact that if a site is in the infinite cluster it must, by definition, be magnetic. The remainder of this section is concerned with the derivation of $D^E(v, q)$, and the next section to the series $\Sigma_i D_i^F(v, q)$.

The $D^E(v, q)$ factors may be obtained in the form of a simple generating function. The site itself must be magnetic if v is to be greater than or equal to one, giving rise to a term p. It then has Q surrounding sites, where Q is the coordination number of the lattice under consideration. Each of these may increase the valency of the chosen site by one (with probability p) or leave it unchanged (with probability q). Therefore $D^E(v, q)$ may be obtained as a binomial-type distribution

$$D^E(v, q) = \text{coefficient of } X^v \text{ in } (1-q)[q+(1-q)X]^Q \tag{2.2}$$

for v between 0 and Q.

It is of interest to note that $D^E(v, q)$ is a function only of q and Q, independent of the lattice structure. The results obtained for the entire system are therefore identical for the triangular and simple cubic lattices. Only the contribution of the finite clusters $D_i^F(v, q)$ introduces the lattice dimensionality into the problem, and into the series $D^I(v, q)$.

3. Site valency for finite clusters

The calculation of $D_i^F(v, q)$ for a particular lattice requires the classification of all clusters of size N according to

(i) the number of isolating sites required to surround the cluster;

(ii) the number of sites with valencies 1 to Q in the cluster.

All clusters which can be drawn on the lattice, and are identical under consideration of (i) and (ii), are summed to give their 'embedding' count. Classification of clusters according to (i) alone has been considered in a series of papers by Sykes and Gaunt (1976), Sykes and Glen (1976) and Sykes *et al* (1976a, b, c).

The series $\Sigma_i D_i^F(v, q)$ may be calculated from these embedding counts:

$$\sum_i D_i^F(v, q) = \sum_i (1-q)^{N_i} q^{P_i} E_i D_i(v) = \sum_r a_r(v) q^r \tag{3.1}$$

where N_i is the number of sites forming cluster i, P_i is the number of perimeter sites isolating cluster i, E_i is the embedding count of cluster i and $D_i(v)$ is the number of sites of valency v in cluster i. The coefficients $a_r(v)$ for the SQ, PT and SC lattices, based on clusters of up to 13, 10 and 9 sites, respectively, are presented in tables 1, 2 and 3. Limits may be easily placed on the accuracy of the number of terms using the perimeter results of Sykes and Glen (1976) and Sykes *et al* (1976b). For example, on the SQ lattice the first entry of fourteen sites (D_{14}) is at q^{13}, and hence our results are correct up to q^{12}.

4. Bond valency for the entire system

Using the same approach as in § 2, we define a quantity $B^E(l, m, q)$, denoting the probability of a bond in the entire system having sites of valencies l and m at either end.

Table 1. $a_r(v)$ for a simple quadratic lattice.

r \ v	1	2	3	4
6	4			
7	0	4		
8	8	2	4	1
9	−24	30	0	−1
10	112	−22	48	20
11	−276	110	−40	−28
12	876	−46	320	199

Table 2. $a_r(v)$ for a triangular lattice.

r \ v	1	2	3	4	5	6
8	6					
9	−12	6				
10	24	−3	6			
11	−42	3	0	6		
12	84	21	8	−3	6	1
13	−144	−45	−8	27	−12	−1
14	288	189	120	−69	66	12

Table 3. $a_r(v)$ for a simple cubic lattice.

r \ v	1	2	3	4	5	6
10	6					
11	−12					
12	6					
13	24	12				
14	−66	−33				
15	78	27	8			
16	6	81	−20			
17	−198	−291	0	12		
18	390	510	112	−57	6	1
19	−474	−588	−256	105	−36	−7
20	684	588	264	42	90	21
21	−1302	−912	−12	−678	−48	−23
22	1818	1623	−220	1947	−384	−55
23	−606	−699	−56	−3651	1554	315
24	−4878	−5568	288	5622	−3696	−839

This leads to the equation

$$B^{\mathrm{I}}(l, m, q) = \frac{B^{\mathrm{E}}(l, m, q) - \Sigma_i B_i^{\mathrm{F}}(l, m, q)}{(1-q)^2} \tag{4.1}$$

with obvious notation for finite cluster contributions.

Again, generating functions may be obtained for the $B^{\mathrm{E}}(l, m, q)$, but now the lattice structure must be considered. For the loose-packed quadratic and simple cube lattices

we have a straightforward generalisation of (2.2). $B^{E}(l, m, q)$ is given by the coefficient of $X^{l}Y^{m}$ (which is the same as the coefficient of $X^{m}Y^{l}$) in

$$\tfrac{1}{2}Q(1-q)^{2}XY[q+(1-q)X]^{Q-1}[q+(1-q)Y]^{Q-1} \tag{4.2}$$

multiplied by a factor of two if $l \neq m$ to account for degeneracy.

For the triangular lattice, however, the generalisation is not so immediate. There are two sites which, if chosen, are capable of increasing the valencies of both sites under consideration. We now find that $B^{E}(l, m, q)$ for the triangular lattice is given by the coefficient of $X^{l}Y^{m}$ or $X^{m}Y^{l}$ in

$$3(1-q)^{2}XY[q+(1-q)XY]^{2}[q+(1-q)X]^{3}[q+(1-q)Y]^{3} \tag{4.3}$$

again multiplied by two if $l \neq m$ to account for degeneracy. Equations (2.2), (4.2) and (4.3), in fact, lead to the same results as Domb (1971) but presented, we feel in a more compact notation.

Table 4. $b_r(l, m)$ for a simple quadratic lattice.

r \ l, m	1,1	1,2	1,3	1,4	2,2	2,3	2,4	3,3	3,4	4,4
6	2									
7	−4	8								
8	2	−12	12	4	8					
9		12	−24	−12	8	24	8			
10		−8	68	52	−38	28	12	18	12	2
11		32	−160	−148	120	−44	−8	28	28	8
12		−32	476	432	−276	280	212	58	88	32

5. Bond valency for finite clusters

The calculation of $B_i^{F}(l, m, q)$ for a particular lattice is similar to that of $D_i^{F}(v, q)$ requiring the classification of all clusters of size N according to

(i) the number of isolating non-magnetic sites required to surround the cluster;

(ii) the number of particular bond valencies within the cluster.

All clusters which can be drawn on the lattice, and are identical under consideration of (i) and (ii), are summed to give their 'embedding count'. The series $\Sigma_i B_i^{F}(l, m, q)$ may be calculated from these results:

$$\sum_i B_i^{F}(l, m, q) = \sum_i (1-q)^{N_i} q^{P_i} E_i B_i(l, m)$$

$$= \sum_r b_r(l, m) q^{r} \tag{5.1}$$

where $B_i(l, m)$ is the number of bonds with valencies l, m in cluster i.

Results obtained for the SQ, PT and SC lattices are presented in tables 4, 5 and 6. These are based upon consideration of all clusters of up to sizes 11, 9 and 8, respectively. By consideration of the more compact clusters of larger sizes, we have produced results accurate to the powers given. In all cases the $B^{F}(1, 1)$ term has been included for completeness, but is however a finite rather than an infinite series with a probability equal to that of an isolated bond. This ensures that $B^{1}(1, 1, q) = 0$, since the probability of finding an isolated bond in the IC must be zero.

Table 5. $b_r(l, m)$ for a triangular lattice.

r \ l, m	1,1	1,2	1,3	1,4	1,5	1,6	2,2	2,3	2,4	2,5	2,6	3,3	3,4	3,5	3,6	4,4	4,5	4,6	5,5	5,6	6,6
8	3																				
9	−6						6														
10	3	18					−18	12				3									
11		−54	12				30	−12	12			−6	12								
12		108	−30	6			21	−24	−12	12		42	−30	18	6	12					
13		−186	60	−18			−6	144	0	−36		−138	126	−60	−18	−24	36	12			
14		330	−96	54			114	−306	6	120		399	−333	228	66	51	−90	−18	27	18	3

Table 6. $b_r(l, m)$ for a simple cubic lattice.

r \ l,m	1,1	1,2	1,3	1,4	1,5	1,6	2,2	2,3	2,4	2,5	2,6	3,3	3,4	3,5	3,6	4,4	4,5	4,6	5,5	5,6	6,6
10	3																				
11	−6																				
12	3																				
13		24																			
14		−66																			
15		54	24																		
16		66	−60				48														
17		−246	0	48			−168														
18		42	240	−228	30	6	291	96													
19		−216	−456	420	−180	−42	−324	−312													
20		−120	252	−24	450	126	330	444	192			48									
21		396	80	−1656	−360	−162	−540	−228	−1056	120	24	−144									
22		−276	−1260	4608	−1110	−144	741	48	2988	−810	−186	180	192								
23		168	1320	−8100	4860	1146	498	−576	−5496	2790	720	−24	−1008	120	24						
24		−1410	−984	11868	−11322	−3030	−4452	−96	7476	−6378	−1823	62	2760	−780	−180	192					

6. Mean cyclomatic number

The cyclomatic number of any cluster with n sites and e connections is defined by

$$c = e - n + 1. \tag{6.1}$$

The average number of connections in an n-site cluster, $\langle e \rangle$, may be obtained from the D factors by multiplying by the appropriate number of connections and summing over all possible values for finite clusters:

$$\langle e \rangle = \frac{n}{2(1-q)} \sum\!\!\!\!\!\!\diagup \sum_{v=1}^{Q} v D_i^{\mathrm{F}}(v, q) \tag{6.2}$$

where $\sum\!\!\!\!\!\!\diagup$ denotes summation over all clusters of size n. For the entire system

$$\langle e \rangle = \frac{n}{2(1-q)} \sum_{v=1}^{Q} v D^{\mathrm{E}}(v, q) = \tfrac{1}{2} npQ. \tag{6.3}$$

Dividing both sides of (6.1) by n, and taking the limit of large n, we obtain for the mean cyclomatic number per site:

$$\frac{\langle c \rangle}{n} = \frac{\langle e \rangle}{n} - 1 \tag{6.4}$$

which may range from 0 to a value $c_{\max} = (\frac{1}{2}Q) - 1$. Dividing (6.4) by $c_{\max}$ gives us a normalised value:

$$\frac{\langle c \rangle}{n c_{\max}} = \frac{1}{c_{\max}} \left(\frac{\langle e \rangle}{n} - 1 \right). \tag{6.5}$$

Combining (6.5), (6.3), (6.2) and (2.1) we can obtain a normalised value for the mean cyclomatic number per site for the IC. This we shall term lambda after Domb and Stoll (1977) and call the coefficient of compactness. (Note that in their case for the SQ lattice $c_{\max} = 1$.) Lambda is given by

$$\lambda = \frac{1}{2(1-q)(\frac{1}{2}Q - 1)} \sum_{v=1}^{Q} v \left(D^{\mathrm{E}}(v, q) - \sum_i D_i^{\mathrm{F}}(v, q) \right). \tag{6.6}$$

In order to calculate the exact value of λ the sum over i in (6.6) should extend over all finite clusters, giving a set of infinite series in q. Since only so many of these terms can be calculated, approximations have to be formed to the series behaviour at higher orders of q. Padé approximants (e.g. Baker 1970) are used for this purpose, and fortunately give reasonable agreement between themselves. Typical plots of λ as a function of p are given in figures 1, 2 and 3 for the lattices under consideration.

The graphs are seen to be linear over a large part of the range $p > p_c$, and correspond to the equation

$$\lambda = (\tfrac{1}{2}Q - 1)^{-1}(\tfrac{1}{2}pQ - 1). \tag{6.7}$$

This equation is, in fact, identical with that obtained for the behaviour of the entire system by using (6.3) and (6.5), and we can see equivalent behaviour for the triangular and simple cubic lattices ($Q = 6$) in the region $p > 0{\cdot}65$. As p is reduced to p_c the graphs begin to depart from straight-line behaviour, levelling out, and rapid oscillations set in when p is reduced below p_c—a non-physical situation.

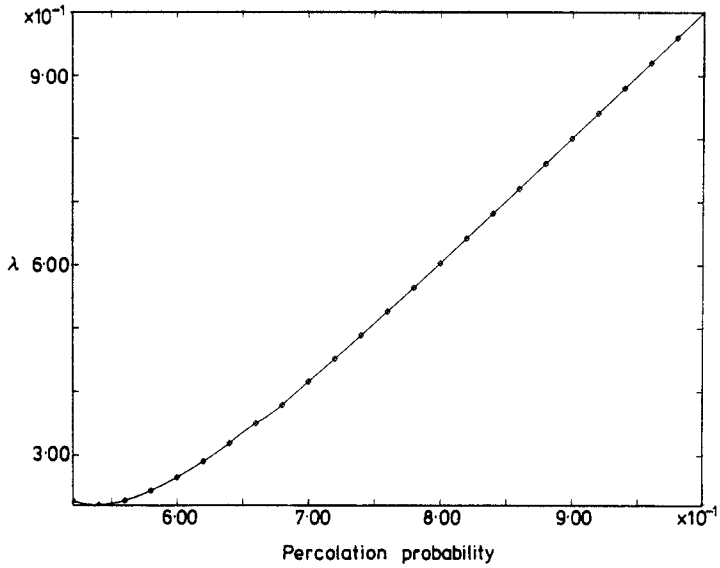

Figure 1. Coefficient of compactness λ plotted against percolation probability p for the infinite cluster on the SO lattice.

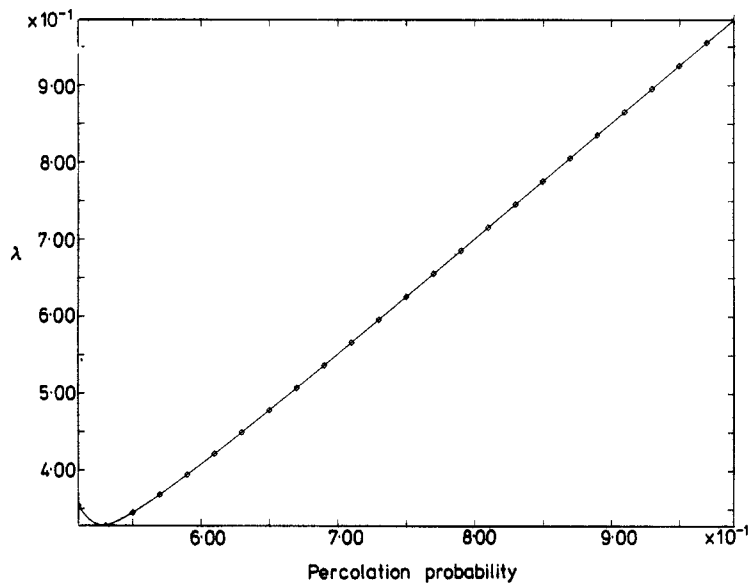

Figure 2. Coefficient of compactness λ plotted against percolation probability p for the infinite cluster on the PT lattice.

Our results for the SQ lattice may be compared with those of Domb (1978), obtained by Monte Carlo techniques, and are seen to be in reasonable agreement. We can see that near p_c λ is a small fraction of its maximum value of unity, corresponding to the idea of ramified clusters playing an important role in percolation theory. Furthermore, the infinite cluster is seen to dominate the system over a large part of its range, since its average behaviour is very close to the average for the entire system.

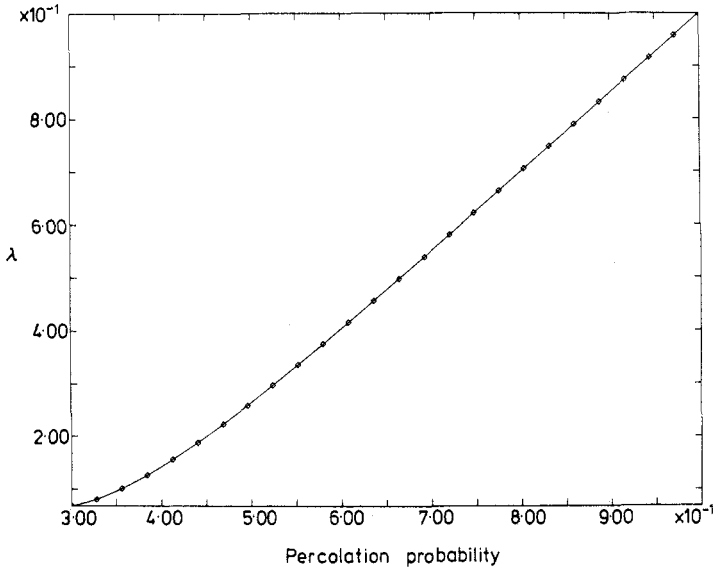

Figure 3. Coefficient of compactness λ plotted against percolation probability p for the infinite cluster on the SC lattice.

7. Low-temperature expansion

We now proceed to outline the techniques for deriving a low-temperature expansion for the free energy of the IC in a site-dilute ferromagnet. The mean number of spins in the IC is given by

$$M = NP(p) \tag{7.1}$$

where $P(p)$ is the well known percolation probability. The Hamiltonian of the IC is given by

$$H_M^{IC} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - mH \sum_{i=1}^{M} \sigma_i \tag{7.2}$$

in which $\langle ij \rangle$ runs over all nearest-neighbour spins in the IC and $\sigma_i = \pm 1$.

The corresponding partition function can be obtained:

$$Z_M^{IC} = \sum\!\!\!\!\!\!\diagup \prod_{\langle ij \rangle} \exp(J\sigma_i\sigma_j/kT) \prod_{\langle i \rangle} \exp(mH\sigma_i/kT) \tag{7.3}$$

where $\sum\!\!\!\!\!\!\diagup$ is the sum over all spin states. Dividing out from this the spin-ordered state:

$$Z_M^{IC} = \mu^{-M/2} Z^{-MQ'/4} \Lambda_M(\mu, z) \tag{7.4}$$

where $\mu = \exp(-2mH/kT)$, $Z = \exp(-2J/kT)$ and Q' is the mean coordination number of the IC derived from the relationship

$$Q' = \sum_{v=1}^{Q} v\, D^1(v, q). \tag{7.5}$$

$\Lambda_M(\mu, z)$ is an expansion formed by considering the energy change, from the ordered state, obtained by successively 'flipping' spins into orientations anti-parallel to the

external field. The first term in the series is unity, corresponding to no overturned spins. The next term arises from flipping one spin. There are M spins to choose from, each with a probability $D^{\mathrm{I}}(v, q)$ of having valency v and thus changing the energy of v interactions. Its contribution is therefore given by

$$\mu M\Big(\sum_{v=1}^{Q} D^{\mathrm{I}}(v, q) z^{v}\Big). \tag{7.6}$$

When two spins are overturned, there are two cases to be considered, depending on whether or not the spins are adjacent.

7.1. Adjacent spins

If we overturn adjacent spins of degree l and m, then we will effectively change the sign of $l+m-2$ interactions. The probability of choosing two such spins is given by $(MQ'/2)B^{\mathrm{I}}(l, m, q)$, giving rise to a term

$$\mu^{2}\frac{MQ'}{2}\Big(\sum_{\substack{l,m=1\\ m\geq l}}^{Q} B^{\mathrm{I}}(l, m, q) z^{l+m-2}\Big). \tag{7.7}$$

7.2. Disjoint spins

Now the sign of $l+m$ interactions will be changed. The number of such spins is found by subtracting the number of adjacent spins from the total number of pairs, and we find the terms

$$\begin{aligned} &\mu^{2} M z^{l+m}\Big(MD(l, q)D(m, q)-\frac{Q'}{2}B^{\mathrm{I}}(l, m, q)\Big) && l\neq m\\ &\mu^{2} M z^{2l}\Big(\frac{D(l, q)(D(l, q)-1)}{2}-\frac{Q'}{2}B^{\mathrm{I}}(l, l, q)\Big) && l=m. \end{aligned} \tag{7.8}$$

$\Lambda_{M}(\mu, z)$ therefore becomes

$$\begin{aligned} 1+\mu M\Big(\sum_{v=1}^{Q} D^{\mathrm{I}}(v, q) z^{v}\Big)+\mu^{2}\Big[&\Big(\frac{MQ'}{2}\sum_{\substack{l,m=1\\ m\geq l}} B^{\mathrm{I}}(l, m, q) z^{l+m-2}\Big)(1-z^{2})\\ &+\Big(M^{2}\sum_{\substack{l,m=1\\ m>l}}^{Q} D^{\mathrm{I}}(l, q)D^{I}(m, q) z^{l+m}\Big)\\ &+\Big(\frac{M}{2}\sum_{l=1}^{Q} D^{\mathrm{I}}(l, q)\,(MD^{\mathrm{I}}(l, q)-1) z^{2l}\Big)\Big]+\mathrm{O}(\mu^{3}). \end{aligned} \tag{7.9}$$

Taking the logarithm of (7.9) we arrive at an expression for the free energy per site of the infinite cluster

$$\begin{aligned} F &= -\frac{kT}{M}\ln Z_{M}^{\mathrm{IC}}\\ &= -mH-\frac{Q'}{2}J-\frac{1}{kT}\Big\{\mu\Big(\sum_{v=1}^{Q} D^{\mathrm{I}}(v, q) z^{v}\Big) \end{aligned}$$

$$+\frac{\mu^2}{2}\left[Q'(1-z^2)\left(\sum_{\substack{l,m=1\\ m\geqslant l}} B^{\mathrm{I}}(l,m,q)z^{l+m-2}\right)\right.$$

$$\left.-\sum_{v=1}^{Q} D^{\mathrm{I}}(v,q)z^{2v}\right]+\mathrm{O}(\mu^3)\Bigg\} \tag{7.10}$$

and we arrive at a series in μ, whose coefficients are themselves series in q. Our present series are too short to come to any conclusions concerning the behaviour of (7.10), but it is hoped they will be lengthened.

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