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LETTER TO THE EDITOR

Exact enumeration approach to fractal properties of the percolation backbone and $1/\sigma$ expansion

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Abstract. An exact enumeration approach is developed for the backbone fractal of the incipient infinite cluster at the percolation threshold. We use this approach to calculate exactly the first low-density expansion of $L_{BB}(p)$ for arbitrary system dimensionality d, where $L_{BB}(p)$ is the mean number of backbone bonds and p is the bond occupation probability. Standard series extrapolation methods provide estimates of the fractal dimension of the backbone for all d; these disagree with the Sierpinski gasket model of the backbone. We also calculate the first low-density expansions of $L_{min}(p)$ and $L_{red}(p)$ which are, respectively, the mean number of bonds in the minimum path between i and j and the mean number of singly connected ('red') bonds.

How can one describe the flow of fluid in random porous media? This important question has long eluded explanation. Recently, considerable attention has been focused on the utility of fractals as models of random media. In particular, the topology of the network that exists just at the onset of fluid flow has been modelled by percolation theory. Bonds are considered intact if fluid can flow through them. When the fraction of bonds is small, the system consists of many small finite clusters. However, as the bond fraction approaches a critical value p_c the clusters grow large and ramified until at p_c fluid can flow. If we consider the network of intact bonds right at p_c, there will be a subset of bonds that carry fluid ('backbone' bonds) and a remainder that does not ('dangling ends'). The structure of the backbone remains an important open question. Two models of the backbone have been discussed in the literature. In one (Gefen *et al* 1981), the backbone is replaced by a d-dimensional Sierpinski gasket. In the other (Stanley 1977, Coniglio 1981, 1982, Pike and Stanley 1981, Stanley and Coniglio 1983), the backbone is considered to consist of an alternating sequence of singly connected ('red') bonds and multiply connected ('blue') bonds; these are shown in colour as figure 5 of Hamann (1983).

The advantage of the Sierpinski gasket model of the backbone is that one can calculate exactly its fractal dimension, $D_B = \ln(d+1)/\ln 2$. Hence it is important to obtain estimates of D_B for the actual backbone of percolation clusters. Thus far, the only efforts have been Monte Carlo simulations in $d = 2$, 3 for the backbone order parameter exponent β_B; however, the order parameter is extremely difficult to calculate by Monte Carlo methods (Kirkpatrick 1978, Li and Streider 1982). Also, a limited attempt has been made to estimate the field-like scaling power y_h by large-cell

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position-space renormalisation group; however, this work was limited to $d = 2$. The Sierpinski gasket model gives reasonable quantitative values for $d = 2$, 3 but not for higher d. For this and other reasons, it is highly desirable to have calculations of d_f for the backbone for general d, in order that one can better assess the relative merits of various models of backbone topology. To this end, here we present an exact enumeration approach for the backbone fractal, and calculate the first ten terms in the low-density expansions for *arbitrary* d. We shall see that these ten terms behave sufficiently smoothly with increasing order that extrapolations to obtain the asymptotic behaviour can be made (table 1).

Table 1. Critical exponents characterising the backbone of the incipient infinite cluster in percolation. The basic quantities calculated are ζ_B and ζ_{min}, since $\zeta_{red} = 1$ for all d (Coniglio 1982). In order to obtain the exponent for the derived quantities $L_{BB}(p)$ and $L_{min}(p)$, we need γ_p, which is also tabulated. Finally, to obtain the backbone fractal dimension, D_B, we need ν.

	γ_p	ν	ζ_B	ζ_{min}	$D_B = \frac{\rho_B}{\nu}$	$D_B = \frac{\ln(d+1)}{\ln 2}$
$d = 2$	$\frac{43}{18}$[a]	$\frac{4}{3}$[a]	2.40 ± 0.05[j]	1.38 ± 0.1[j] 1.49 ± 0.02[i]	1.80 ± 0.04[j]	1.585[f]
$d = 3$	1.73 ± 0.03[b] 1.66 ± 0.07[c] 1.66[d]	0.88 ± 0.02[b]	1.61 ± 0.07[j]	1.18 ± 0.07[j]	1.83 ± 0.08[j]	2.000[f]
$d = 4$	1.48 ± 0.08[e] 1.40[d] 1.41 ± 0.25[c]	0.7[h]	$1.32^{+0.10}_{-0.15}$	1.03 ± 0.08[j]	$1.89^{+0.14}_{-0.21}$	2.322[f]
$d = 5$	1.16[d] 1.18 ± 0.07 1.25 ± 0.15	0.6[h]	$1.16 \bullet 0.1$[j]	1.02 ± 0.1[j]	1.93 ± 0.16[j]	2.585[f]
$d = 6 - \varepsilon$	$1 + \frac{1}{7}\varepsilon + 0.046\varepsilon^2$	$0.5 + \frac{5}{84}\varepsilon$	$1 + \frac{1}{7}\varepsilon$[g] $+ 0.025\varepsilon^2$	—	$2 + 0.0476\varepsilon$ $+ 0.0186\varepsilon^2$	—
$d = 6$	1.00[a]	0.500[a]	1.02 ± 0.02[j]	1.02 ± 0.02[j]	2.04 ± 0.04[j]	2.807[f]

[a] Exact.
[b] Gaunt and Sykes (1983).
[c] Gaunt *et al* (1976).
[d] Fisch and Harris (1978).
[e] Gaunt *et al* (1976).
[f] Gefen *et al* (1981).
[g] Harris and Lubensky (1983).
[h] Stauffer (1979).
[i] Pike and Stanley (1981).
[j] This work.

Since the 'thermal' scaling power $y_T = 1/\nu$ is the same for the backbone as for the full cluster (Shlifer *et al* 1979), it is sufficient to calculate only one exponent in addition to ν. Since low-density expansions are generally more accurate than high-density expansions for the same effort, we focus our attention on the exponent ζ_B rather than on β_B.

In order to define clearly our approach, it is useful to review how one may calculate the exponent γ for the full cluster (Essam 1971, Dunn *et al* 1975). The pair connectedness P_{ij} is defined to be the probability that sites i and j are connected,

$$P_{ij} = [\nu_{ij}]_{\text{config}}, \tag{1a}$$

where $\nu_{ij}=1$ if sites i and j are connected (belong to the same cluster) and $\nu_{ij}=0$ otherwise. The square brackets denote a configurational average over all 2^N configurations of an N-bond system. For example, for $d=1$, $P_{ij}=p^{|i-j|}$. The mean cluster size or 'susceptibility' is given by the fluctuation relation

$$S(p)=\chi_P(p)=\sum_{ij} P_{ij}\sim\varepsilon^{-\gamma}, \tag{1b}$$

where $\varepsilon=(p_c-p)/p_c\to 0^+$ and γ is the mean-size critical exponent. For $d=1$, the known result (Reynolds *et al* 1977) $S(p)=(1+p)/(1-p)\sim\varepsilon^{-1}$ follows immediately from (1*b*).

These ideas can be extended to other quantities (Fisch and Harris 1978, Coniglio 1982). Thus for the backbone we may define

$$B_{ij}=[b_{ij}\nu_{ij}] \tag{2a}$$

where b_{ij} is the number of backbone bonds connecting sites i and j. For $d=1$, $B_{ij}=|i-j|p^{|i-j|}$. In analogy with equation (1*b*), we may define the 'backbone susceptibility'

$$\chi_{BB}(p)=\sum_{ij} B_{ij}. \tag{2b}$$

For $d=1$, we have $\chi_{BB}(p)=2p/(1-p)^2$.

Below p_c, the mean number of backbone bonds L_{BB} connecting two sites i and j that are separated a distance of the order of the correlation length is (Coniglio 1982)

$$L_{BB}(p)=\sum_{ij} B_{ij}/\sum_{ij} P_{ij}\sim\varepsilon^{-\zeta_B}, \tag{3}$$

which defines the critical exponent ζ_B for the backbone.

Using the cumulant method, we have developed a low-density expansion for $\chi_{BB}(p)$ in the form

$$\chi_{BB}(p)=\sum_{n=1}^{\infty} B_n(d)p^n, \tag{4}$$

and have evaluated the coefficients $B_n(d)$ in closed form for all d for $1\leqslant n\leqslant 10$. To this end, we have generalised the inclusion–exclusion principle for the pair connectedness function to the backbone. The generalisation arises from the fact that the number of backbone bonds between sites i and j, like the pair connectedness P_{ij}, is independent of any 'dangling ends'. Therefore we only need self-avoiding walks (SAWs) and loop diagrams that are constructed by the union of SAWs between i and j. Thus for any graph G the average B_{ij} is given by

$$B_{ij}=\sum_{g} C(g)E(g)p^{b(g)}, \tag{5a}$$

where the summation runs over all subgraphs of the graph G, $E(g)$ is the embedding constant, $b(g)$ is the number of bonds of g, and the cumulant $C(g)$ satisfies the recursive relation (Essam 1971, Fisch and Harris 1978)

$$C(g)=V(g)-\sum_{g'} C(g'). \tag{5b}$$

Here $V(g)$ is the value of g, while g' are the subgraphs of g.

For example, consider the simple four-bond graph $G(\square)$, where the crosses denote sites i and j. Applying (5), we find

$$B_{ij} = C\left(\square^{\times}_{\times\square}\right)p^4 + 2C\left(\square^{\times}_{\times}\right)p^2$$

$$= \left[V\left(\square^{\times}_{\times\square}\right) - 2V\left(\square^{\times}_{\times}\right)\right]p^4 + 2V\left(\square^{\times}_{\times}\right)p^2$$

$$= [4 - 2\times 2]p^4 + [2\times 2]p^2. \tag{6a}$$

Had we assigned the value $V(g) = 1$ for each graph, then we would have recovered the usual inclusion–exclusion principle,

$$P_{ij} = [1 - 2\times 1]p^4 + [2\times 1]p^2 = -p^4 + 2p^2. \tag{6b}$$

For the infinite lattice, with two fixed sites i and j, there are of course an *infinite* number of SAWs joining i and j (unless the lattice has directed bonds). Therefore we cannot perform an exact calculation, but instead must perform an expansion in increasing powers of p, by including in the calculation graphs with increasing numbers of bonds and multiplying the contribution of each graph by the appropriate lattice embedding constant (Fisch 1977). Thus the initial terms in this expansion are

$$\chi_{BB}(p) = C_{BB}(\times - \times)[2d]p + C_{BB}(\times - \cdot - \times)[(2d)(2d-1)]p^2$$
$$+ C_{BB}(\times - \cdot - \cdot - \times)[(2d)(2d-1)^2]p^3$$
$$+ C_{BB}(\times - \cdot - \cdot - \cdot - \times)[2d(2d-1)^3 - 4d(d-1)]p^4$$
$$+ \left[4C_{BB}\left(\begin{smallmatrix} \cdot & - & \times \\ | & & | \\ \times & - & \cdot \end{smallmatrix}\right) + 8C_{BB}\left(\begin{smallmatrix} \cdot & - & \cdot \\ | & & | \\ \times & - & \times \end{smallmatrix}\right)\right]d(d-1)p^4. \tag{7a}$$

Here the backbone cumulant $C_{BB}(g)$ for a diagram g is given by

$$C_{BB}(g) = V(g) - \sum_{g' \in g} C_{BB}(g'). \tag{7b}$$

The expansion (7) increases rapidly in complexity, but the requisite diagrams and lattice embedding constants are known through order p^{10} (Baker *et al* 1967, Fisch 1977). Therefore it is necessary only to apply the recursive relation (6) to each graph g and then to calculate the number of backbone bonds in each subgraph g'. The general-d expressions in the form of (7) are given in table 2.

We find that the coefficients $B_n(d)$ in the series for the backbone $\chi_{BB}(p)$ are of the same form as the coefficients in the series for mean size $S(p)$,

$$B_n(d) = \sum_{k=1}^{n} W_{n,n-k+1}\binom{d}{k}. \tag{8}$$

The (d-independent) coefficients $W_{n,n-k+1}$ are given in table 2(a) up to $n = 10$. We find for the first two coefficients the simple results

$$W_{n1} = n2^n n! \tag{9a}$$

$$W_{n2} = 2n(n-1)^2 2^{n-2}(n-1)! \tag{9b}$$

$$W_{n3} = \tfrac{1}{3}n2^{n-4}(n-2)!(6n^4 - 40n^3 + 96n^2 - 128n + 126) + 24(n-3)2^{n-4}(n-2). \tag{9c}$$

Table 2. General-d low-density series. (a) The coefficients $W_{n,n-k+1}$ appearing in the expression (8) for $B_n(d)$, which in turn are the coefficients in the expansion (4) for the backbone susceptibility. The leading coefficients W_{nm} are given in equations (9a), (b), and (c). (b) The analogous coefficients from which one constructs the coefficients $M_n(d)$ of the mean number of bonds in the minimum path of (10b). The leading coefficients are the same as (9a) and (9b), while (9c) is replaced by $W_{n3}=3^{-1}n2^{n-4}(n-2)!(6n^4-40n^3+96n^2-128n+126)+8\times 2^{n-4}(n-3)(n-2)!$ (c) The analogues appearing in $R_n(d)$ of (11b). Again, the leading coefficients are the same as (9a) and (9b), while (9c) is replaced by $W_{n3}=3^{-1}2^{n-4}(n-2)!\times(6n^4-40n^3+96n^2-128n+126)$.

	1	2	3	4	5	6	7	8	9	10
(a)										
1	2									
2	4	16								
3	6	96	144							
4	8	384	1 728	1 536						
5	10	1 352	13 296	30 720	19 200					
6	12	4 272	84 672	381 312	576 000	276 480				
7	14	12 992	488 496	3 810 048	10 440 960	11 612 160	4 515 840			
8	16	37 040	2 638 608	33 713 664	149 160 960	288 368 640	252 887 040	82 575 360		
9	18	104 016	13 716 048	276 767 616	1 855 644 480	5 546 880 000	8 227 215 360	5 945 425 920	1 672 151 040	
10	20	274 504	68 358 432	2 151 197 568	21 096 368 000	91 577 917 440	204 343 050 240	245 114 634 240	150 493 593 600	37 158 912 000
(b)										
1	2									
2	4	16								
3	6	96	144							
4	8	352	1 728	1 536						
5	10	1 224	12 912	30 720	19 200					
6	12	3 508	78 816	376 704	576 000	276 480				
7	14	10 748	444 648	3 694 848	10 379 520	11 612 160	4 515 840			
8	16	27 052	2 303 880	32 024 256	146 956 800	287 447 040	252 887 040	82 575 360		
9	18	79 076	11 790 120	258 819 648	1 809 174 720	5 502 274 560	8 211 732 480	5 945 425 920	1 672 151 040	
(c)										
1	2									
2	4	16								
3	6	96	144							
4	8	336	1 728	1 536						
5	10	1 160	12 720	30 720	19 200					
6	12	3 144	76 032	374 400	576 000	276 480				
7	14	9 716	424 200	3 639 552	10 348 800	11 612 160	4 515 840			
8	16	22 592	2 154 048	31 241 472	145 889 280	286 986 240	252 887 040	8 257 360		
9	18	68 436	10 948 536	250 681 536	1 787 313 600	5 480 524 800	8 203 991 040	594 525 920	1 672 151 040	
10	20	143 080	51 796 080	1 902 043 520	20 037 046 400	89 773 286 400	202 916 044 800	244 681 113 600	150 493 593 600	37 158 912 000

In order to form the function $L_{BB}(p)$ of (3), we must also obtain general-d expressions for the mean-size function $S(p)$ for bond percolation with *site* counting (as opposed to *bond* counting, as in the conventional series expansions). Fortunately, Fisch and Harris (1978) tabulate the needed results.

The resulting series were analysed for $d = 2-6$ by the usual extrapolation procedures. We found that Padé approximants provided the most consistent estimates of the backbone exponent ζ_B defined in (3), and the results are shown in table 1. Table 1 also shows $D_B = \zeta_B/\nu$, the fractal dimension of the backbone. For comparison, we include the prediction $D_B = \ln(d+1)/\ln 2$ of the Sierpinski gasket model. We see that the discrepancy is most serious for large d.

The same procedure developed above for the number of backbone bonds B_{ij} can be readily extended to the *minimum* number of bonds M_{ij} (Middlemiss *et al* 1980, Pike and Stanley, 1981), where $M_{ij} = [m_{ij}\nu_{ij}]$ in analogy to (2a). The general-d results are given in table 2(b) while table 1 also gives the results of extrapolation procedures for the exponent ζ_{min} defined through

$$L_{min}(p) = \sum_j M_{ij} / \sum P_{ij} = \chi_{min}(p)/\chi_p(p) \sim \varepsilon^{-\zeta_{min}}, \tag{10a}$$

where

$$\chi_{min}(p) = \sum_{n=1}^{\infty} M_n(d) p^n. \tag{10b}$$

Similarly we can define

$$L_{red}(p) = \sum_j R_{ij} / \sum P_{ij} = \chi_{red}(p)/\chi_p(p) \sim \varepsilon^{-\zeta_{red}}, \tag{11a}$$

$$\chi_{red}(p) = \sum_{n=1}^{\infty} R_n(d) p^n, \tag{11b}$$

where $R_{ij} = [r_{ij}\nu_{ij}]$ is the number of singly connected ('red') bonds or links between sites i and j. Pike and Stanley (1981) found that $L_{red}(p)$ diverges at p_c, contrary to some intuitive expectations, and Coniglio (1981, 1982) proved rigorously that $\zeta_{red} = 1$ for all spatial dimensionalities d. The proof was based on the 'Lemma' that $L_{red}(p) = p\,(\mathrm{d}/\mathrm{d}p)\log S(p)$. We find that Coniglio's lemma holds 'term-by-term' in the sense that for each graph in the low-density series expansion,

$$L_{ij} = p(\mathrm{d}/\mathrm{d}p)\log P_{ij}. \tag{12}$$

In table 2, we tabulate the general-d results for the function $\Sigma_j R_{ij}$.

Although less reliable than direct analysis, an approximation to the functions $\chi_{BB}(p)$, $\chi_{min}(p)$ and $\chi_{red}(p)$ may be obtained by deriving expansions in the variable $1/\sigma$, where $\sigma = 2d-1$. Following the procedure used for $\chi_p(p)$ (Gaunt and Ruskin 1978), we find to $O(1/\sigma^2)$,

$$\chi_{BB} = \chi_{BB}^{CT} + (-5x^2/(1-x)^3 + x/(1-x)^2 - 18x/(1-x) + 7x + x^2)\sigma^{-2} + \ldots, \tag{13a}$$

$$\chi_{min} = \chi_{min}^{CT} + (-5x^2/(1-x)^3 - 3x/(1-x)^2 - 6/(1-x) - x - 3x^2)\sigma^{-2} + \ldots, \tag{13b}$$

$$\chi_{red} = \chi_{red}^{CT} + [-5x^2/(1-x)^3 - 5x/(1-x)^2 - 5x - 5x^2]\sigma^{-3} + \ldots, \tag{13c}$$

where $x = \sigma p$. Following the procedure used in deriving

$$\chi_p^{CT}(p) = 1 + (\sigma^{-1} + 1) \sum_{r=1}^{\infty} (\sigma p)^r = (1+p)/(1-\sigma p), \tag{14a}$$

we obtain

$$\chi_{BB}^{CT} = \chi_{min}^{CT} = \chi_{red}^{CT} = (1+\sigma^{-1}) \sum_{r=1}^{\infty} r(\sigma p)^r = (\sigma+1)p/(1-\sigma p)^2. \tag{14b}$$

In summary, then, we have calculated the first low-density expansions for three quantities characterising the backbone fractal of the incipient infinite cluster at the percolation threshold. These are L_{BB}, L_{min} and L_{red} which, respectively, are the mean number of backbone bonds, the mean length of minimum path, and the mean number of 'red' bonds between sites i and j separated by a correlation length. Extrapolations for the corresponding critical exponents, ζ_{BB} and ζ_{min}, are presented in table 1; ζ_R is known to diverge as $1/\varepsilon$ for all d (Coniglio 1982).

After this work was completed, we received two interesting preprints (Harris 1983, Harris and Lubensky 1983) which apply field-theoretic methods to calculate *one* of these quantities, L_{BB}, as a series in $(6-d)$; for $d > 3$, their results are not inconsistent with ours based on series expansions.

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References

Baker G A, Gilbert H E, Eve J and Rushbrooke G S 1967 *BNL 50053(T-460)* (Brookhaven National Laboratory)
Coniglio A 1981 *Phys. Rev. Lett.* **46** 250
—— 1982 *J. Phys. A: Math. Gen.* **15** 3829
Dunn A G, Essam J W and Ritchie D S 1975 *J. Phys. C: Solid State Phys.* **8** 4219
Essam J W 1971 *J. Math. Phys.* **12** 874
Fisch R 1977 *PhD thesis* University of Pennsylvania
Fisch R and Harris A B 1978 *Phys. Rev.* B **18** 416
Gaunt D S and Ruskin H 1978 *J. Phys. A: Math. Gen.* **11** 1369
Gaunt D S and Sykes M F 1983 *J. Phys. A: Math. Gen.* **16** 783
Gaunt D S, Sykes M F and Ruskin H 1976, *J. Phys. A: Math. Gen.* **9** 1899
Gefen Y, Aharony A, Mandelbrot B B and Kirkpatrick S 1981 *Phys. Rev. Lett.* **47** 1771
Hamann D R 1983 *Phys. Today* **36** [5] 25
Harris A B 1983 *Preprint*
Harris A B and Lubensky T C 1983 *Preprint*
Kirkpatrick S 1978 *AIP conference* **40** 99
Li P S and Streider W 1982 *J. Phys. C: Solid State Phys.* **15** L1235
Middlemiss K M, Whittington S G and Gaunt D S 1980 *J. Phys. A: Math. Gen.* **13** 1835
Pike R and Stanley H E 1981 *J. Phys. A: Math. Gen.* **14** L169
Reynolds P J, Stanley H E and Klein W 1977 *J. Phys. A: Math. Gen.* **11** L203
Shlifer G, Klein W, Reynolds P J and Stanley H E 1979 *J. Phys. A: Math. Gen.* **12** L169
Stanley H E 1977 *J. Phys. A: Math. Gen.* **10** L211
Stanley H E and Coniglio A 1983 in *Percolation Structures and Processes* ed G Deutscher, R Zallen and J Adler (Bristol: Adam Hilger) p 101
Stanley H E, Redner S and Yang Z R 1982 *J. Phys. A: Math. Gen.* **15** L569
Stauffer D 1979 *Phys. Rep.* **54** 1