Series expansion evidence supporting the Alexander–Orbach conjecture in two dimensions

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Abstract. We extend the series expansion of Fisch and Harris for the resistive susceptibility $\chi_R(p)$ by a further six terms on the square lattice. This leads to a more precise estimate of the corresponding exponent $\gamma_R = 3.65 \pm 0.02$. We also obtain the exact relation $\chi_R(p) = 2\mathscr{E}(\tau|F)$, where τ is the sum of the relaxation times for charge diffusion on the cluster containing the origin and the expectation value is subject to the condition that the latter is finite. A known scaling relation for the fracton dimension, D_f, in terms of γ_R and the static exponents is derived without the usual reference to the infinite cluster. Using our estimate of γ_R we find $D_f = 1.334 \pm 0.007$, which is consistent with the AO conjecture $D_f = \frac{4}{3}$. We also note that γ_R is the same for directed and undirected percolation to within the accuracy of our calculations.

1. Introduction

The purpose of this paper is to investigate the conductivity of random-resistor networks in the vicinity of the percolation threshold p_c. Fisch and Harris (1978, referred to as FH below) approached this problem by obtaining low density series expansions for the resistive susceptibility defined by

$$\chi_R(p) = \sum_r R(r, p) \tag{1}$$

where $R(r, p)$ is the mean resistance between the lattice site at an arbitrary chosen origin **0** and the site with vector r, given that both sites are in the same finite cluster. They also defined a resistive length $L_R(p) = \chi_R(p)/S(p)$, where the normalising factor $S(p) = \mathscr{E}(s|F)$. Here s is the size of the cluster containing **0** and the expectation $\mathscr{E}$ is subject to the condition, F, that this cluster is finite (see (20)). The exponents describing the divergence at p_c of χ_R, S and L_R are respectively γ_R, γ and ζ_R ($=\gamma_R - \gamma$).

In scaling theory for percolation (Dunn *et al* 1975) the central quantities are the scaling parameters $\xi(p)$, the connectedness length, and $\mathscr{S}(p)$, a measure of the number of sites in a cluster of linear dimension $\xi(p)$, which diverge at p_c with critical exponents ν and Δ respectively. $\mathscr{S}(p)$ may be defined more precisely by $\mathscr{E}(s^2|F)/\mathscr{E}(s|F)$. In two dimensions there is good evidence (den Nijs 1979, Nienhuis *et al* 1980) that these

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exponents have the exact values $\nu = \frac{4}{3}$ and $\Delta = 2 + \frac{19}{36}$ which we shall use in this work. The percolation probability $P(p)$ is approached from above p_c with exponent given, using hyperscaling, by $\beta = d\nu - \Delta$, where d is the space dimension; also $\gamma = \Delta - \beta$.

According to Skal and Shklovskii (1975) and de Gennes (1976) the dynamic exponent t which describes the vanishing of the conductivity $\Sigma(p)$ of the infinite cluster as $p \to p_c$ from above is given by

$$t = (d-2)\nu + \zeta_R. \tag{2}$$

This relation enabled FH to obtain the first estimate of t by series expansion methods. Gefen *et al* (1983) defined a further dynamic exponent θ for charge diffusion on percolation clusters such that the time scale $\mathcal{T}(p)$ for diffusion over a distance of order $\xi(p)$ is given by

$$\mathcal{T}(p) \sim \xi(p)^{2+\theta}. \tag{3}$$

Fick's law for non-random media corresponds to $\theta = 0$. Using the Einstein relation between diffusion and conduction on the infinite cluster they obtained the scaling relation

$$\theta = (t - \beta)/\nu. \tag{4}$$

Alexander and Orbach (1982, referred to as AO below) introduced the fracton dimension D_f (we use the notation of Alexander 1983) which in the present context may be defined by

$$\mathcal{T}(p) \sim \mathcal{S}(p)^{2/D_f}. \tag{5}$$

The definition may be motivated by the fact that a cluster of uniform density would have linear dimension $\sim \mathcal{S}^{1/d}$ and (5) with $D_f = d$ would then be Fick's law. Comparison with (3) gives

$$D_f = 2D/(2+\theta) \tag{6}$$

where D is the fractal dimension Δ/ν, and combining this with (4) AO found

$$D_f = 2(d\nu - \beta)/(t - \beta + 2\nu). \tag{7}$$

Using (2) and the hyperscaling relation for β we find

$$D_f = 2/(1 + \zeta_R/\Delta). \tag{8}$$

In § 3 we give an independent argument for this relation which refers only to finite clusters and is therefore valid below as well as above p_c. The argument will also avoid the use of hyperscaling and the Einstein relation.

The advantage of using D_f rather than θ as the critical exponent for charge diffusion lies in the conjecture of AO that D_f (and hence the relation between $\mathcal{T}$ and $\mathcal{S}$) is independent of d and equal to its value $\frac{4}{3}$ on the Bethe lattice. This is reasonable on the basis that $\mathcal{S}$, but not ξ, incorporates the variation of fractal dimension with d. The value $D_f = \frac{4}{3}$ was consistent with the numerical data at the time; however the AO conjecture inspired a number of recent more accurate Monte Carlo calculations (see table 1) the results of which suggest that, for $d = 2$, $\frac{4}{3}$ is wrong (however it lies within 1% of the observed values). Also current ε expansion results about $d = 6$ (Harris *et al* 1984) are inconsistent with the AO conjecture.

We have extended the 10th-order expansion of FH for $\chi_R(p)$ on the square lattice by a further six terms (table 2). Analysis of this series leads to an estimate of γ_R and hence ζ_R (table 1) of accuracy comparable to that obtained by the above Monte Carlo

Table 1. Summary of estimates of ζ_R and D_f the square lattice bond problem.

Reference	$\zeta_R\ (=t)$	D_f
Alexander and Orbach (1982)	1.263 88	4/3
Our calculation	1.26 ± 0.02	1.334 ± 0.007
Hong *et al* (1984)	1.293 ± 0.012	1.323 ± 0.004
Zabolitzky (1984) (Monte Carlo method)	1.297 ± 0.007	1.322 ± 0.003
Herrmann *et al* (1984) (transfer matrix method)	1.303 ± 0.014	1.320 ± 0.005
Lobb and Frank (1984)	$1.297^{+0.007}_{-0.004}$	$1.322^{+0.001}_{-0.003}$

Table 2. $\chi_R(p) = 4p + 24p^2 + 108p^3 + 362p^4 + 1220p^5 + 3398p^6 + 2\sum_{n=7}^{\infty} a_n p^n$.

n	a_n(Num)	a_n(Den)
7	77 896	15
8	190 748	15
9	4312 604	115
10	67 668 856	805
11	6071 648 971	24 955
12	4828 591 206 345	9442 972
13	1510 174 078 768 384 784 429	1023 115 770 360 684
14	482 303 050 428 087 010 967 529 511	168 262 715 788 986 334 230
15	444 197 575 004 259 426 177 746 638 313 824 078	50 695 608 356 180 386 483 307 488 065
16	268 782 103 489 806 974 480 277 855 715	18 509 481 186 104 307 221 989 677
	656 058 101 816 325 067 199 210 653	003 086 133 373 297 404 240 300

work. The value $D_f = 1.334 \pm 0.007$ calculated from ζ_R using (8) appears to reopen the question of the validity of the AO conjecture. Also the recent conjecture of Sahimi (1984) $t = 1 + 2\beta = 1.277 \ldots$ falls just within our estimated range. On the other hand the conjecture of Aharony and Stauffer (1984), $\zeta_R = \nu = 1.333 \ldots$, for $d = 2$, seems unlikely to be true. It has been noted by one of us (FMB) and independently by Adler (private communication) that our result $\gamma_R = 3.65 \pm 0.02$ for undirected percolation and the value (Bhatti and Essam 1984) $\gamma_R = 3.654 \pm 0.017$ for directed percolation clusters are the same to the accuracy of the calculations. If this were an exact result then it would provide a second estimate of $D_f = 1.333 \pm 0.007$. The γ_R's in three dimensions (Adler 1985, Bhatti 1984) are less well determined due to the large uncertainty in the estimates of p_c; however the values for directed and undirected clusters are quite close. In the remainder of the paper we give details of the series derivation and analysis and also present a derivation of (8).

2. Series derivation and analysis

2.1. Derivation of low density series for $\chi_R(p)$

It is possible to reformulate the 'cumulant' expansion method used by FH in the form

$$\chi_R(p) = \sum_m R(g_m) N_m(p) p^{e_m} \tag{9}$$

where e_m is the number of edges in the graph g_m. $N_m(p)$ is an infinite power series with integer coefficients and $R(g_m)$ is the sum of R_{ij}, the resistance between vertices i and j of g_m, over all vertex pairs. Only graphs in the form of generalised chains need be included in the list; up to order 16 there are 9725 of these. For each graph, R was computed by two separate programs, one of which solved Kirchoff's equations by a graphical technique which gave the exact rational values and the other calculated the eigenvalues of the dynamical matrix of the graph (see below) using a standard package. The $N_m(p)$ depend on the lattice and a good check on the calculation of these for the square lattice was available since keeping the same N_m and replacing $R(g_m)$ by other functions gave the known mean number and mean size expansions (Sykes *et al* 1981) (the latter was known only to order 15).

2.2 Estimation of γ_R

We have used two methods to analyse the $\chi_R(p)$ series, both of which allow for corrections to scaling. In the Baker–Hunter method (1973) the series is transformed according to $p = p_c(1 - e^{-x})$, where $p_c = \frac{1}{2}$, and denoting by b_k the coefficient of x^k in the resulting expansion, Padé approximants are calculated for the series $f(x)$ having general term $k! b_k$. Now if $\chi_R(p)$ was of the form

$$\chi_R(p) = \sum_{i=1}^{n} A_i(1 - p/p_c)^{-\gamma_i} \tag{10}$$

then the parameters $1/\gamma_i$ and A_i would be given exactly by the poles and residues of the $[m - 1/m]$ sequence of approximants to $f(x)$. The extent to which the method works in practice will depend on the position and relative strength of the non-physical singularities which are also present in $\chi_R(p)$. Table 3 gives the estimates of $\gamma_R = \gamma_1$. We notice that the values of γ_R obtained from the last four terms of the series are well converged and that there is a general downward trend as the number of terms is increased. These data suggest $\gamma_R = 3.65 \pm 0.02$ and that any change due to further extension of the series is unlikely to be in the upward direction. We also estimate the first correction-to-scaling exponent $\gamma_1 - \gamma_2 = \Delta_1 = 1.24 \pm 0.06$, in good agreement with the value obtained from other $d = 2$ percolation series (Adler *et al* 1982).

   In the method of Adler *et al* (1982, 1983) Padé approximants are formed to $z(1 - x)$ times the Dlog of the series obtained by the transformation $p = p_c[1 - (1 - x)^{1/z}]$ where z is a parameter. The resulting approximants, for given z, evaluated at $x = 1$ give

Table 3. Estimates of γ_R using the Baker–Hunter method.

Term	$[N/N+2]$	$[N/N+1]$	$[N/N]$	$[N+1/N]$	$[N+2/N]$
10		3.68		*	
11	3.67		3.67		*
12		3.68		*	
13	3.64		3.64		*
14		3.64		3.64	
15	3.64		3.64		*
16		3.65		3.66	

* Only one pole on the positive real axis.

estimates of γ_R. In an ideal situation with only one confluent singularity and no non-physical singularities all approximants would give γ_R exactly whenever $z = \Delta_1/k$, $k = 1, 2, \ldots$. In practice the harmonics $k \geq 2$ are rarely observed and even analytic confluent terms can influence the convergence; values of z are sought which optimise the apparent convergence. The value $z = 1$ corresponds to the standard biased Dlog method. Adler *et al* (1982) analysed the three mean size expansions for bond percolation on the square lattice and found $\gamma = 2.375 \pm 0.015$, $\Delta_1 = 1.25 \pm 0.15$, in good agreement with $\gamma = 2 + \frac{7}{18} = 2.3888\ldots$ (see above). Standard Padé analysis of these same series had given values which were mutually inconsistent and as high as 2.42. The fact that the technique of Adler *et al* removes this inconsistency is a strong point in its favour. Recently Adler (1985) has analysed the ten-term expansion of FH for $\chi_R(p)$. She argues that the same value of Δ_1 should be used as for the mean size series and finds, using the above range of Δ_1, $\gamma_R = 3.70 \pm 0.20$. Our sixteen-term series gives much better convergence (see table 4) and we find that as z varies from 1.1 to 1.4, γ_R decreases from 3.67 to 3.63. This is the same range as we found using the Baker–Hunter method. Various sets of approximants were tried and RMS deviation δ quoted in the table is based on the [5/7], [7/5], [5/8], [6/7], [7/6], [5/9], [7/7] and [8/6] approximants. These were chosen on the basis of having no defects in the range of z considered. The variation of the estimated γ_R with z is an order of magnitude greater than δ. Again we note the downward trend with increasing length of series.

Table 4. Estimates of γ_R using the Adler *et al* (1983) method.

z	γ_R	δ	z	γ_R	δ
1.00	3.679	0.0027	1.25	3.650	0.0037
1.05	3.673	0.0023	1.30	3.644	0.0044
1.10	3.667	0.0022	1.35	3.639	0.0052
1.15	3.661	0.0025	1.40	3.633	0.0061
1.20	3.657	0.0030			

2.3. The conductive susceptibility

We have also extended the FH series for the conductive susceptibility, $\chi_C(p)$, on the square lattice to sixteen terms (table 5) and corrected a significant error in the eighth term. The only change required in the computer program was to replace R_{ij} (§ 2.10) by the conductance, $C_{ij} = 1/R_{ij}$, between sites i and j of the cluster. The recent analysis of Adler (1985) gave the exponent $\gamma_C = 0.98 \pm 0.04$. The results obtained using the method of Adler *et al* on the extended series are still not well converged and we show in table 6 the values for a set of non-defective approximants with $z = 1.25$ which use between 11 and 16 terms of the series. We estimate $\gamma_C = 1.1 \pm 0.1$ which takes account of the variation of z between 1.1 and 1.4 and the upward trend with increasing length of series. The value obtained from γ_R using the scaling relation $\gamma_C = 2\gamma - \gamma_R$ is 1.13 ± 0.02 which is consistent with the less accurate direct estimate. The Baker–Hunter method applied to this series is less successful and fails to give Δ_1 consistently. The value of γ_C is higher than that of Adler but still falls below the range obtained from γ_R.

Table 5. $\chi_C(p) = 4p + 6p^2 + 12p^3 + 25p^4 + 2\sum_{n=5}^{\infty} c_n p^n$.

n	c_n
5	0.242 095 238 095 238 095 238 095 24D + 02
6	0.488 060 606 060 606 060 606 060 60D + 02
7	0.964 138 528 138 528 138 528 138 52D + 02
8	0.193 673 990 542 747 882 344 337 98D + 03
9	0.385 979 260 240 082 864 424 457 15D + 03
10	0.772 277 170 106 625 935 335 221 58D + 03
11	0.154 707 797 596 630 339 462 145 81D + 04
12	0.309 257 794 363 586 442 138 865 59D + 04
13	0.623 711 963 833 191 277 510 219 67D + 04
14	0.122 315 936 007 545 586 435 763 30D + 05
15	0.257 672 913 297 331 778 637 009 46D + 05
16	0.469 291 090 501 607 828 814 246 94D + 05

Table 6. Estimates of γ_C using the method of Adler *et al* (1983) with $p_c = 0.5$ and $z = 1.25$.

Padé	5/4	4/5	6/4	4/6	5/6	4/7	5/7	7/6	4/9	9/5	8/6	5/9
γ_C	0.97	1.02	1.09	0.98	0.99	0.99	0.98	0.99	1.09	1.34	1.12	1.11

3. Scaling theory for diffusion on percolation clusters

We conclude by deriving equation (8). It is sufficient to show that

$$\mathcal{T}(p) \sim L_R(p)\mathcal{S}(p) \tag{11}$$

since (8) follows by combining (11) with the definition (5) and comparing exponents. Relation (11) was postulated by one of us (Essam 1980) on the basis that $\mathcal{S}(p)$ is a measure of the electrical capacity of a cluster with linear dimension of order $\xi(p)$. However we shall obtain below the exact equation

$$\chi_R(p) = 2\mathcal{E}(\tau|F) \tag{12}$$

where τ is the sum of relaxation times for charge diffusion on the cluster c_0 containing 0 and the expectation $\mathcal{E}$ is calculated subject to the condition F that c_0 is finite. Following Dunn *et al* (1975) we show that this equation leads to (11).

Consider a cluster with s sites, bond resistance r and $s \times s$ adjacency matrix A. The dynamical matrix is $B = D - A$ where D is a diagonal matrix with $D_{kk} = d_k$, the valence of site k in the cluster. Solving Kirchoff's equations, the resistance R_{ij} between sites i and j is given by

$$R_{ij} = r \det[B(i,j)]/\det[B(j)] \tag{13}$$

where $B(j)$ is the matrix B with the jth row and column deleted and $B(i, j)$ has the ith and jth rows and columns deleted. Since $\det(B) = 0$ we have

$$\det(B - \lambda I) = -\lambda(\lambda_1 - \lambda)(\lambda_2 - \lambda)\dots(\lambda_{s-1} - \lambda)$$
$$= -b_1\lambda + b_2\lambda^2 \dots + b_{s-1}(-\lambda)^{s-1} + (-\lambda)^s. \tag{14}$$

where λ_k is the kth non-zero eigenvalue of B and b_i is the sum of the determinants of all principal submatrices of B having $s - i$ rows and columns, thus

$$b_1 = \sum_{j=1}^{s} \det[B(j)] \qquad b_2 = \sum_{[i,j]} \det[B(i,j)] \qquad (15)$$

where the second sum is over all subsets of two sites of c. Hence

$$\sum_{[i,j]} R_{ij} = rsb_2/b_1 = rs \sum_{j=1}^{s-1} (1/\lambda_k) \qquad (16)$$

where we have used the fact that $\det B(j)$ is independent of j and found b_2/b_1 by equating coefficients of λ and λ^2 in (14). Now attach capacity C to each site of the lattice and place charge Q on the above cluster. By charge conservation at site i we have

$$\frac{dq_i}{dt} = -(1/rC) \sum_{k=1}^{s-1} B_{ik}q_k \qquad (17)$$

and ignoring possible degeneracy problems

$$q_i = \frac{Q}{s} + \sum_{k=1}^{s-1} a_{ik} \, e^{-t/\tau_k} \qquad (18)$$

where the a_{ik} depend on the initial charge distribution and $\tau_k = rC/\lambda_k$, the relaxation time of the kth normal mode. Therefore if $C = 1$

$$\sum_{[i,j]} R_{ij} = s \sum_{i=1}^{s-1} \tau_i = s\tau. \qquad (19)$$

It was shown by Dunn *et al* (1975) that if $\dot{X}_c(i)$ is a property of the cluster c, relative to some site $i \in c$, which is independent of the position of c relative to the lattice then

$$p_F \mathscr{E}(X|F) = \lim_{L \to \infty} (1/N_L) \left\langle \sum_{c \in \mathscr{C}_L(\omega)} \sum_{i \in c} X_c(i) \right\rangle \qquad (20)$$

where on the LHS $X = X_c(0)$, the average on the RHS is over all configurations ω of the infinite lattice and $\mathscr{C}_L(\omega)$ is the set of all clusters enclosed by a cube of side L centred on 0 and containing N_L sites. p_F is the probability that c_0 is finite. If $X_c(i) = s_c$, the number of sites in c, independently of i, then we obtain

$$p_F S(p) = \lim_{L \to \infty} (1/N_L) \left\langle \sum_{c \in \mathscr{C}_L(\omega)} s_c^2 \right\rangle \qquad (21)$$

but if $X_c(i) = \Sigma_{j \in c} R_{ij}$ then

$$p_F \chi_R(p) = \lim_{L \to \infty} (1/N_L) \left\langle \sum_{c \in \mathscr{C}_L(\omega)} \sum_{i,j \in c} R_{ij} \right\rangle$$

$$= \lim_{L \to \infty} (2/N_L) \left\langle \sum_{c \in \mathscr{C}_L(\omega)} s_c \tau_c \right\rangle \qquad (22)$$

where we have used (19) applied to c. Using (20) again with $X_c = \tau_c$ gives (12). Equations (21) and (22) suggest the scaling relations

$$S(p) \sim \mathscr{N}(p)\mathscr{S}(p)^2 \qquad \text{and} \qquad \chi_R(p) \sim \mathscr{N}(p)\mathscr{S}(p)\mathscr{T}(p) \qquad (23)$$

which combine to give (11). Here $\mathscr{N}(p)$ is the number of clusters per site having of order $\mathscr{S}(p)$ sites.

Acknowledgments

Note added in proof. The earlier work of Sahimi *et al* (1983) gives $t = 1.264 \pm 0.054$ in agreement with the AO conjecture.

References

Adler J 1985 *J. Phys. A: Math. Gen.* **18** 307-14
Adler J, Moshe M and Privman V 1982 *Phys. Rev.* B **26** 1411-5
—— 1983 *Ann. Israel Phys. Soc.* **5** 397-423
Aharony A and Stauffer D 1984 *Phys. Rev. Lett.* **52** 2368-70
Alexander S 1983 *Ann. Israel Phys. Soc.* **5** 149-65
Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625-31
Baker G A and Hunter D L 1973 *Phys. Rev.* B **7** 3377-92
Bhatti F M 1984 *J. Phys. A: Math. Gen.* **17** 1771-3
Bhatti F M and Essam J W 1984 *J. Phys. A: Math. Gen.* **17** L67-73
de Gennes P G 1976 *J. Physique Lett.* **37** L1
den Nijs M P M 1979 *J. Phys. A: Math. Gen.* **12** 1857-68
Dunn A G, Essam J W and Loveluck J M 1975 *J. Phys. C: Solid State Phys.* **8** 743-50
Essam J W 1980 *Rep. Prog. Phys.* **43** 833-912 (we refer here to an unpublished preprint of chapter 9)
Fisch R and Harris A B 1978 *Phys. Rev.* B **18** 416-20
Gefen Y, Aharony A and Alexander S 1983 *Phys. Rev. Lett.* **50** 77-80
Harris A B, Kim S and Lubensky T C 1984 *Phys. Rev. Lett.* **53** 743-6
Herrmann H J, Derrida B and Vannimenus J 1984 *Phys. Rev.* B **30** 4080-2
Hong D C, Havlin S, Herrmann H J and Stanley H E 1984 *Phys. Rev.* B **30** 4083-6
Lobb C J and Frank D J 1984 *Phys. Rev.* B **30** 4090-2
Nienhuis B, Riedel E K and Schick M 1980 *J. Phys. A: Math. Gen.* **13** L189-92
Sahimi M 1984 *J. Phys. A: Math. Gen.* **17** L601-7
Sahimi M, Hughes B D, Scriven L E and Davis H T 1983 *J. Phys. C: Solid State Phys.* **16** L521-7
Skal A S and Shklovskii B I 1975 *Sov. Phys.-Semicond.* **8** 1029-32
Sykes M F, Gaunt D S and Glen M 1981 *J. Phys. A: Math. Gen.* **14** 287-93
Zabolitzky J G 1984 *Phys. Rev.* B **30** 4077-9