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A note on the convergence of the series expansion for the mean cluster size in random mixtures

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Abstract. New data for the site percolation problem on the simple quadratic lattice are given. It is concluded that the critical concentration p_c does not correspond to the radius of convergence of the series expansion for the mean cluster size.

Series expansions have been used to estimate the critical probability p_c for both site and bond percolation problems. A general survey of the literature and a description of the problem is given in the recent review by Shante and Kirkpatrick (1971). The series method originated from studies of the threshold concentration of dilute ferromagnets (Elliott *et al* 1960, Heap 1963); it was suggested by Domb and Sykes (1961) that the critical (threshold) concentration could be obtained from a direct study of random mixtures. Specifically, Domb and Sykes derived series expansions for the mean size of clusters in ascending powers of the concentration p. For the simple quadratic site problem they obtained:

$$\begin{aligned} S(p) &= \sum a_n p^n \\ &= 1+4p+12p^2+24p^3+52p^4+108p^5+224p^6 \\ &\quad +412p^7+844p^8+1528p^9+\ldots . \end{aligned} \tag{1}$$

The mean size, $S(p)$, is the mean size of finite clusters containing a randomly chosen site (for a discussion see Fisher and Essam 1961); this quantity, which is a weighted average, becomes infinite at the critical concentration p_c.

Domb and Sykes made the hypothesis that the critical concentration corresponded to the radius of convergence of (1). On physical grounds it is to be supposed that $S(p)$ has no singularities on the positive real axis for $p < p_c$; the hypothesis relies on the assumption that the coefficients a_n are all positive. Sykes and Essam (1964) added the coefficient $+3152p^{10}$ to (1) and undertook a detailed analysis; they found the evidence inconclusive but reasonably consistent with the assumption that near p_c,

$$S(p) \sim \frac{1}{(p_c-p)^{j+1}} \tag{2}$$

with $j \simeq 1{\cdot}375$. The techniques employed drew their inspiration largely from somewhat analogous series analysis problems that arise in the Ising problem and excluded volume problem. (For a recent treatment see Sykes *et al* 1972a.)

Using special methods developed by one of us (JLM), combined with the graph theoretical results of Essam and Sykes (1966), we have added a further seven coefficients to $S(p)$:

$$+5036p^{11}+11\,984p^{12}+15\,040p^{13}+46\,512p^{14}+34\,788p^{15}+197\,612p^{16}+4036p^{17}+\ldots \quad (3)$$

In the figure we illustrate the successive ratios μ_n, defined by

$$\mu_n = \frac{a_n}{a_{n-1}} \quad (4)$$

and the quantity

$$\rho_n = \left(\frac{a_n}{a_{n-2}}\right)^{1/2} \quad (5)$$

introduced by Sykes and Essam to smooth the oscillations. After $n = 10$, the last value available in earlier investigations, a rapid *alternating* divergence becomes manifest; indeed one can suppose with some confidence that the coefficient a_{19} will be *negative*.

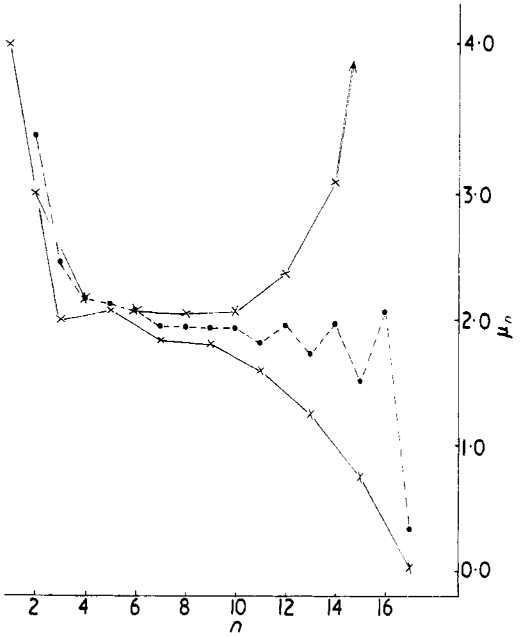

Figure 1. Analysis of the coefficients of $S(p)$. Crosses and full lines: successive ratios μ_n. Circles and broken lines: the quantity ρ_n.

The alternation strongly suggests the presence of a singularity closer to the origin than the physical divergence of $S(p)$; p_c cannot therefore be identified with the radius of convergence of (1).

To investigate the singularities of $S(p)$ we have studied the Dlog Padé approximants. Our tentative conclusions are that the closest singularity occurs on the *negative* real axis at $p^* \simeq -0{\cdot}324 \pm 0{\cdot}010$ with a very weak singularity; a pair of singularities in the complex plane is also indicated at $p^{**} \simeq -0{\cdot}20 \pm 0{\cdot}45\mathrm{i}$ (modulus $\sim 0{\cdot}49$), again closer than the physical singularity. We present the diagonal and paradiagonal sequences for the closest singularity in table 1, and for the physical singularity in table 2. From table 2 it will be seen that the successive approximations are not especially well behaved; they appear consistent with the estimates in table 3, taken from the literature.

Table 1. Dlog Padé analysis: closest singularity. Estimates of p^* (and the corresponding exponent) from the poles and residues of the Padé approximants to Dlog $S(p)$

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	−0·27823(−0·2640)	−0·51229(−1·7774)	none
3	none	none	none
4	−0·55298(−0·9107)	−0·35498(−0·0884)	−0·32019(−0·0412)
5	−0·31382(−0·0345)	−0·32277(−0·0441)	−0·32239(−0·0436)
6	−0·32235(−0·0436)	−0·32286(−0·0442)‡	−0·32193(−0·0431)§
7	−0·32174(−0·0428)†	−0·32240(−0·0437)§	−0·32118(−0·0422)‡§
8	−0·31741(−0·0381)‡	−0·33401(−0·0618)§	

† Defect on positive axis. ‡ Defect on negative axis. § Defect in complex plane.

Table 2. Dlog Padé analysis: closest singularity on positive real axis. Estimates of p_c (and the corresponding exponent $-j-1$) from the poles and residues of the Padé approximants to Dlog $S(p)$

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	1·07823(−5·3360)	0·23518(−0·0679)	none
3	0·48627(−1·0693)	0·72897(−5·1579)	0·31647(−0·0581)
4	0·56034(−1·7139)	0·58972(−2·1632)	0·57972(−1·9701)
5	0·58210(−2·0211)	0·57787(−1·9286)	0·57670(−1·8953)
6	0·57701(−1·9053)	0·57781(−1·9272)‡	0·58233(−2·0092)§
7	0·57026(−1·6938)†	0·57825(−1·9372)§	0·57974(−1·9714)‡§
8	0·58151(−2·0135)‡§	0·58560(−2·1174)§§	

† Defect on positive axis. ‡ Defect on negative axis. § Defect in complex plane.

Table 3. Estimates for p_c for the simple quadratic problem

Source	Method	p_c
Frisch *et al* (1961)	Monte Carlo	0·581 ± 0·015
Dean (1963)	Monte Carlo	0·580 ± 0·018
Sykes and Essam (1964)	Series (ratio method)	0·580 ± 0·020
Sykes and Essam (1964)	Series for matching lattice	0·590 ± 0·010
Dean and Bird (1957)	Monte Carlo	0·591 ± 0·001
Neal (1972)	Monte Carlo	0·590 ± 0·005

We are confronted with a situation where the dominant asymptotic singularity is very weak compared to a second singularity which is further from the origin. This does not invalidate the investigation of Sykes and Essam; it does however imply that additional coefficients cannot be used to estimate p_c with increasing precision by the ratio method. Estimates for the parameter j are likely to be unreliable; indeed it is for this that table 2 is least consistent with their conclusions. A somewhat similar situation has been encountered previously in other problems; by Domb *et al* (1965) for the susceptibility of the Heisenberg model and by Gaunt (1967) for the lattice gas problem. A theoretical discussion is given by Gaunt and Guttmann (1973).

Critical indices such as j for the percolation problem have application to the theory of scaling (see Essam 1972 for a detailed review); they seem likely to be more accessible by series methods than by Monte Carlo techniques although the latter give good estimates for p_c. We have some evidence that expansions for $S(p)$ for other lattices in two and three dimensions do not converge up to p_c; we do not present any as we are undertaking a comprehensive revision of the problem for bond and site mixtures in two and three dimensions.

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References

Dean P 1963 *Proc. Camb. Phil. Soc.* **59** 397–410
Dean P and Bird N F 1967 *Proc. Camb. Phil. Soc.* **63** 477–9
Domb C, Dalton N W, Joyce G S and Wood D W 1965 *Proc. Int. Conf. on Magnetism, Nottingham* 1964 (London: The Institute of Physics and the Physical Society) pp 85–7
Domb C and Sykes M F 1961 *Phys. Rev.* **122** 77–8
Elliott R J, Heap B R, Morgan D J and Rushbrooke G S 1960 *Phys. Rev. Lett.* **5** 366
Essam J W 1972 *Phase Transitions and Critical Phenomena* vol 2, ed C Domb and M S Green (New York: Academic Press) pp 197–270
Essam J W and Sykes M F 1966 *J. math. Phys.* **7** 1573–81
Fisher M E and Essam J W 1961 *J. math. Phys.* **2** 609–19
Frisch H L, Sonnenblick E, Vyssotosky V A and Hammersley J M 1961 *Phys. Rev.* **124** 1021–2
Gaunt D S 1967 *J. chem. Phys.* **46** 3237–59
Gaunt D S and Guttmann A J 1973 *Phase Transitions and Critical Phenomena* vol 3, ed C Domb and M S Green (New York: Academic Press) pp 181–243
Heap B R 1963 *Proc. Phys. Soc.* **82** 252–63
Neal D G 1972 *Proc. Camb. Phil. Soc.* **71** 97–106
Shante V K S and Kirkpatrick S 1971 *Adv. Phys.* **20** 325–57
Sykes M F and Essam J W 1964 *Phys. Rev.* **133** A310–5
Sykes M F, Gaunt D S, Roberts P D and Wyles J A 1972a *J. Phys.* A: *Gen. Phys.* **5** 624–39, 640–52
Sykes M F, Guttmann A J, Watts M G and Roberts P D 1972b *J. Phys.* A: *Gen. Phys.* **5** 653–60