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Percolation processes in two dimensions IV. Percolation probability

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Abstract. New series data are examined for the percolation probability $P(p)$ for site and bond mixtures in two dimensions. It is concluded that the data are reasonably consistent with the hypothesis that $P(p) \simeq B(q_c - q)^{\beta}$ as $q \to q_c-$ with β a dimensional invariant, $\beta = 0{\cdot}138 \pm 0{\cdot}007$ in two dimensions. Estimates of the critical amplitude B are also given. Series data for the mean cluster size $S(p)$ in the high density region are examined and it is tentatively concluded that $S(p) \simeq C'(q_c - q)^{-\gamma'}$ as $q \to q_c-$ and that the data are not inconsistent with the hypothesis $\gamma' = \gamma$.

1. Introduction

In this paper we examine new series data for the percolation probability and mean cluster size in the high density region $(p > p_c)$ for site and bond mixtures in two dimensions. We have introduced the problem in companion papers (Sykes and Glen 1976, Sykes *et al* 1976a, b, to be referred to as I–III); the new data are given in III (appendix). Explicitly we investigate the hypothesis (Rudd and Frisch 1970, Sykes *et al* 1974) that

$$P(p) \simeq B(q_c - q)^{\beta}, \qquad q \to q_c- \tag{1.1}$$

and

$$S(p) \simeq C'(q_c - q)^{-\gamma'}, \qquad q \to q_c-. \tag{1.2}$$

The investigation of (1.1) by Rudd and Frisch was inconclusive and dependent on the various methods of analysis employed.

We have found the high density series to be poorly behaved, particularly for $S(p)$. If q_c, and therefore the extrapolation range, is small only a few coefficients are available; if q_c is large more coefficients are available but the extrapolation range is correspondingly large. We have found it very difficult to draw precise conclusions and have therefore confined our present account to a brief summary of the standard Padé approximant analysis.

2. Series analysis

In this section we use Padé approximants to study the high density expansions for the percolation probability and mean size. The procedure has been described in detail by Gaunt and Guttmann (1974) in their review of series analysis techniques in general.

Only one point requires further discussion. The series for $P(p)$ begins like

$$P(p)=1-q^{\theta}-\ldots$$

where $\theta=\sigma+1$ for the site problem, $\theta=2\sigma$ for the bond problem and $\sigma+1$ equals the lattice coordination number. Hence

$$(\mathrm{d}/\mathrm{d}q)\ln P=-\theta q^{\theta-1}-\ldots$$

so that the first non-zero coefficient corresponds to a relatively high power of the expansion variable. In such cases it seems sensible to examine the $[n+j/n]$ Padé approximants for $j=0, \pm 1$ to the series for both $(\mathrm{d}/\mathrm{d}q)\ln P$ and $q^{-(\theta-1)}(\mathrm{d}/\mathrm{d}q)\ln P$. For the latter function this corresponds to the $[n+j/n]$ approximants to the series for $(\mathrm{d}/\mathrm{d}q)\ln P$, with $j=\theta-2, \theta-1, \theta$. In general we have found this sequence of diagonals to converge slightly better.

On forming Dlog Padé approximants to the series for $P(p)$, it is found that the number and location of singularities inside or on the circle $|q|=q_c$ varies widely from problem to problem. However, with the exception of the HC(B) problem, it appears that the dominant singularity always lies on the negative real q axis at $q=-q_0$, say, with $q_0<q_c$. Consequently, the series coefficients ultimately alternate in sign. For the HC(B) problem the physical singularity at $q=q_c$ seems to determine the radius of convergence and correspondingly the series coefficients are all of one sign; although the ratio method (see Gaunt and Guttmann 1974) is applicable in this case, it is not very useful because of interference from a complex conjugate pair of weak singularities which apparently lie on the circle of convergence $|q|=q_c$ in the left half of the q plane.

For series such as these, experience tells us that we should not expect rapid convergence of the approximants in the vicinity of q_c. This is confirmed by the Dlog Padé estimates of q_c and β (given by the poles and residues respectively) for the HC(B), SQ(B), T(B) and T(S) problems, for which q_c is known exactly (see II). The results are presented in tables 1–4 respectively. The last few estimates are reasonably close to the

Table 1. Dlog Padé estimates of q_c (and β) for the honeycomb bond problem.

n	$[n+2/n]$	$[n+3/n]$	$[n+4/n]$
3	—	0·3400 (0·1155)	0·3444 (0·1285)
4	0·3526 (0·1607)	0·3479 (0·1406)	0·3481 (0·1417)
5	0·3481 (0·1415)	0·3479 (0·1407)‡	0·3472 (0·1378)
6	0·3467 (0·1350)	0·3468 (0·1355)	

‡ Defect on negative axis.

Table 2. Dlog Padé estimates of q_c (and β) for the simple quadratic bond problem.

n	$[n+4/n]$	$[n+5/n]$	$[n+6/n]$
3	0·4402 (0·0372)	0·4488 (0·0443)‡	0·4819 (0·0881)
4	—	0·4842 (0·0930)	0·4816 (0·0876)†
5	0·5013 (0·1458)	0·5266 (0·3531)	0·4986 (0·1323)
6	0·5070 (0·1715)	0·5030 (0·1512)	0·5006 (0·1402)‡
7	0·5183 (0·2331)†		

† Defect on positive axis. ‡ Defect on negative axis.

Table 3. Dlog Padé estimates of q_c (and β) for the triangular bond problem.

n	$[n+8/n]$	$[n+9/n]$	$[n+10/n]$
5	0·6106 (0·0433)	0·6127 (0·0456)‡	0·6298 (0·0704)
6	—	—	0·6626 (0·1877)
7	—	—	0·6442 (0·1041)
8	—	0·6496 (0·1238)	0·6538 (0·1444)
9	0·6520 (0·1348)	0·6380 (0·0949)†	0·6566 (0·1615)‡
10	0·6540 (0·1451)	0·6554 (0·1531)‡	

† Defect on positive axis. ‡ Defect on negative axis.

Table 4. Dlog Padé estimates of q_c (and β) for the triangular site problem.

n	$[n+4/n]$	$[n+5/n]$	$[n+6/n]$
4	—	0·4235 (0·0233)§	0·4890 (0·1004)
5	0·5351 (0·4234)§	0·4916 (0·1074)	0·4876 (0·0972)†
6	0·4977 (0·1279)	0·5152 (0·2497)	0·4936 (0·1126)§
7	0·5000 (0·1373)	0·5002 (0·1384)	0·5008 (0·1410)
8	0·4998 (0·1365)†	0·5004 (0·1390)‡	

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

exact value of q_c in all cases, but the sequences exhibit small irregularities with no definite trend. Following the procedure we used in II for analysing the low density mean size series, which exhibited similar behaviour, we plot the residues against the position of their corresponding poles for each of the four problems. As in II, the last few estimates are found to define fairly accurately a single smooth curve for each problem no matter which sequence is chosen. The residue which would be obtained if a pole were located exactly at q_c can then be read off from the plot and in this way we obtain

$$\beta = 0{\cdot}138 \pm 0{\cdot}007 \tag{2.1}$$

as an overall estimate for the four problems. Corresponding results for the HC(S) and SQ(S) problems are consistent with (2.1) only with much larger uncertainties; these arise (*a*) from the uncertainties in q_c (see II) and (*b*) because there are no usable poles having $q \geq q_c$ so that the plots must be extrapolated up to q_c.

Various alternative procedures have also been tried; for example, by evaluating Padé approximants to the series for $(q-q_c)(\mathrm{d}/\mathrm{d}q)\ln P(p)$ at $q=q_c$. The estimates of β so obtained are presented in table 5 for the HC(B) problem and are quite typical. We

Table 5. Padé estimates of β for the honeycomb bond problem using the $(q-q_c)\,(\mathrm{d}/\mathrm{d}q)$ $\ln P(p)$ series and the exact value of q_c.

n	$[n+2/n]$	$[n+3/n]$	$[n+4/n]$
3	0·2834†‡	0·1397	0·1384
4	0·1375	0·1382	0·1390†
5	0·1379‡	0·1380‡	0·1381
6	0·1379†‡	0·1396	

† Defect on positive axis. ‡ Defect on negative axis.

have also analysed the series obtained by transforming to some new expansion variable in which the physical singularity is closest to the origin (see Gaunt and Guttmann 1974) but while finding ample supportative evidence, we have been unable to improve on (2.1) and accordingly adopt it as our final estimate.

We have used the exact or best estimates of q_c together with (2.1) to estimate the critical amplitudes B defined by (1.1). Two methods have been employed: the calculation of the residues at the pole close to p_c of the Padé approximants to the series for $[P(p)]^{-1/\beta}$ and also evaluation of the Padé approximants to the series for $(q_c-q)[P(p)]^{-1/\beta}$ at $q=q_c$. Results obtained by these methods are in good agreement leading to final estimates of B for the bond problems of:

$$B=\begin{cases}1\cdot533\pm0\cdot003 & \text{HC(B)}\\ 1\cdot545\pm0\cdot004 & \text{SQ(B)}\\ 1\cdot600\pm0\cdot003 & \text{T(B)}\end{cases}\qquad(2.2)$$

and for the site problems of:

$$B=\begin{cases}1\cdot530\pm0\cdot009 & \text{HC(S)}\\ 1\cdot530\pm0\cdot015 & \text{SQ(S)}\\ 1\cdot558\pm0\cdot002 & \text{T(S)}.\end{cases}\qquad(2.3)$$

The uncertainties in p_c (where applicable) and in β each introduce additional uncertainties in B of the order of 1% and 3% respectively. (Larger values of B would result from larger values of both p_c and β.) For the bond and site problems the amplitudes are seen to increase monotonically with increasing lattice coordination number; the amplitudes for the HC(S) and SQ(S) problems are probably very close to one another. In addition, it seems that on a given lattice the amplitude for the bond problem is always greater than for the corresponding site problem. All the above features are exhibited by the Bethe approximation (Fisher and Essam 1961); in this approximation the amplitudes for the HC(S) and SQ(S) problems are exactly equal.

Corresponding calculations have been performed on the high density expansions for the mean size. These series are even more poorly behaved than are the series for the percolation probability and the estimation of γ' is very uncertain. An analogous situation arises in the analysis of low temperature expansions for the Ising model. Thus, although the series for the spontaneous magnetization, which is the analogue of the percolation probability (Kasteleyn and Fortuin 1969, Essam 1972), are not particularly well behaved, they do enable estimates of β to be made with reasonable confidence; however, the zero-field susceptibility series which are analogous to the mean size series (Essam 1972) yield only very tentative estimates of γ' (Gaunt and Sykes 1973). Accordingly we give only a very brief account of the analysis for the T(B) problem; the other bond and site problems lead to similar conclusions.

In table 6(a) we give estimates of γ' obtained by evaluating Padé approximants to the series for $(q_c-q)(\mathrm{d}/\mathrm{d}q)\ln S(p)$ at $q=q_c$. These results, which are not well converged, indicate an exponent between 1·25 and 1·75. According to scaling theory (Kasteleyn and Fortuin 1969, Essam and Gwilym 1971) we expect from II that $\gamma'=\gamma\sim2\cdot43$. To study this rather unexpected result further we have investigated the critical behaviour of various functions related to $S(p)$. For example, we note that the

Table 6. Padé estimates of γ' for the triangular bond problem using the (q_c-q) (d/dq) ln $S'(p)$ series and the exact value of q_c. In (*a*) $S'(p)=S(p)$, while in (*b*) $S'(p)=p_f S(p)$.

	(*a*)			(*b*)		
n	$[n-1/n]$	$[n/n]$	$[n+1/n]$	$[n-1/n]$	$[n/n]$	$[n+1/n]$
2	0·9001	1·0634	1·4121	2·0572	1·3072†	2·6634
3	4·0708†	1·2177	1·1987	8·6442†	2·1826	2·1875
4	1·2003	1·2157‡	0·9582†	2·1876	2·1821†	2·1717†
5	1·1150†	1·2673§	1·3942	2·1719†	2·1831	2·2506
6	1·4869	1·3818	1·3972†	2·2574	2·2218	2·3560†
7	1·2311	1·3373	1·3585	3·3361†	2·1337	2·0888
8	1·3849	1·3574	1·3585‡	2·0951	2·1707†	2·0380
9	1·3725‡	1·3322†	1·7459	2·0539	2·0448	2·0358†
10	1·2399†			2·0516‡		

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

definition of $S(p)$ given by III (1.11) contains in the denominator the function p_f with critical behaviour

$$p_f \equiv p(1-P) \sim p_c - p_c B(q_c-q)^{\beta}, \qquad q \to q_c-. \tag{2.4}$$

Hence the function in the numerator of III (1.11) carries the singularity of $S(p)$ as $q \to q_c-$. We have used this function, namely $p_f S(p)$, to calculate alternative Padé estimates of γ' and these are presented in table 6(*b*). These results indicate a much larger exponent around 2·0 to 2·1. Although we still do not have exponent symmetry ($\gamma=\gamma'$), such a relatively small discrepancy could easily disappear if longer series were available. Various methods aimed at improving the rate of convergence have been tried, including transformation of variables, but without notable success.

To estimate the critical amplitudes C', we have assumed exponent symmetry $\gamma=\gamma'$ and followed procedures analogous to those already described for the amplitude B. The convergence is so poor that the following estimates for C/C' should be regarded as order-of-magnitude estimates only:

$$C/C' \simeq 2{\cdot}4 \text{ HC(B)}, \qquad 1{\cdot}9 \text{ SQ(B)}, \qquad 1{\cdot}3 \text{ T(B)} \tag{2.5}$$

and

$$C/C' \sim 3{\cdot}4 \text{ HC(S)}, \qquad 3{\cdot}9 \text{ SQ(S)}, \qquad 2{\cdot}1 \text{ T(S)}. \tag{2.6}$$

In the Bethe approximation $C/C'=1$ for both bond and site problems.

3. Conclusions

The high density expansions are much more difficult to extrapolate than the corresponding low density expansions. While the methods described in III could be used to add one or two more coefficients in all cases, we have not thought this worthwhile because of the poor convergence already experienced. Although we have found it very difficult to draw precise conclusions, all the available data have been found reasonably consistent with the hypothesis that the mean size exponent γ' and percolation probability exponent β are dimensional invariants in two dimensions.

Our final estimate of $\beta = 0{\cdot}138 \pm 0{\cdot}007$ replaces our preliminary estimate of $\beta = 0{\cdot}14 \pm 0{\cdot}03$ for the T(S) problem (Sykes *et al* 1974). The central value of $\beta = 0{\cdot}138$ is very close to $\frac{5}{36} = 0{\cdot}138888\ldots$ but $\frac{1}{7} = 0{\cdot}1428\ldots$ is well within the quoted uncertainties. As usual the uncertainties are not strict error bounds but just represent a subjective assessment of the rate of convergence of the available numerical data (see, for example, Gaunt and Guttmann 1974). With such badly behaved series it is difficult therefore to rule out completely an exponent of about $\frac{1}{8}$, although such a possibility does seem rather unlikely.

We have been unable to estimate the exponent γ' with any precision. Although exponent symmetry $\gamma' = \gamma$ is not ruled out by our results, if it should fail then it seems likely that $\gamma' < \gamma$.

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