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LETTER TO THE EDITOR

The percolation probability for the site problem on the face-centred cubic lattice

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Abstract. The percolation probability for the site problem on the face-centred cubic lattice is investigated by series methods. It is concluded that $P(p)$ vanishes near the critical point like $(p-p_c)^{\beta}$ with $\beta \simeq 0{\cdot}42 \pm 0{\cdot}06$.

In this letter we report a study of series data for the *percolation probability* $P(p)$ for the site problem on the face-centred cubic lattice. Explicity we investigate the hypothesis that in the high density region $p > p_c$,

$$P(p) \simeq B(p-p_c)^{\beta}, \qquad p \to p_c+. \tag{1}$$

The precise determination of β for three-dimensional lattices is of special theoretical interest because of its relevance to studies of scaling law behaviour in random mixtures (Kasteleyn and Fortuin 1969, Essam 1972; for a more general introduction see Shante and Kirkpatrick 1971). A detailed introduction to the series expansion method for percolation problems is given by Sykes and Glen (1976) and Sykes *et al* (1976a, b, c), to be referred to as I–IV. In IV a detailed analysis of series expansions for the percolation probability for site and bond problems on a variety of lattices led to the conclusion that in two dimensions

$$\beta \simeq 0{\cdot}138 \pm 0{\cdot}007. \tag{2}$$

High density expansions for two-dimensional random mixtures were found to be poorly convergent. Using the methods described in III we have derived expansions for the percolation probability for site and bond problems on a variety of three-dimensional lattices and made an extensive numerical analysis of the coefficients. Convergence in general appears to be less rapid in three dimensions and with the data currently available we have only been able to draw firm conclusions in one case: the site problem on the face-centred cubic lattice. For this we estimate as described below that

$$\beta \simeq 0{\cdot}42 \pm 0{\cdot}06. \tag{3}$$

Data for other three-dimensional mixtures are not inconsistent with the hypothesis that β is a dimensional invariant. Just as in the two-dimensional situation it is difficult with such slowly convergent series to rule out the possibility that β could be identical with the corresponding exponent for the spontaneous magnetization of the Ising model ($\beta_{\rm I} = 0{\cdot}125$ for two dimensions, $\beta_{\rm I} = 0{\cdot}3125$ for three dimensions); on the evidence it seems more likely that for random mixtures $\beta > \beta_{\rm I}$, especially in three dimensions.

For the site problem on the face-centred cubic lattice we have derived the expansion

$$\begin{aligned}P(p)=1-q^{12}-12q^{18}+12q^{19}-24q^{22}+12q^{23}-50q^{24}+168q^{25}-222q^{26}+140q^{27}\\ -252q^{28}+558q^{29}-1\,160q^{30}+2\,208q^{31}-2\,625q^{32}+1\,892q^{33}\\ -5\,372q^{34}+16\,440q^{35}-27\,103q^{36}+32\,568q^{37}-39\,336q^{38}\\ +34\,236q^{39}-15\,646q^{40}+88\,122q^{41}-391\,259q^{42}+870\,993q^{43}\\ -1\,268\,634q^{44}+1\,271\,543q^{45}-\ldots\end{aligned} \tag{4}$$

From a detailed analysis (Sykes *et al* to be published) of the corresponding low density expansion for the mean size of finite clusters $S(p)$, we expect that $P(p)$ has its closest singularity on the positive real axis at

$$q=q_c=0\cdot802\pm0\cdot003. \tag{5}$$

This is confirmed by the Padé approximants to the $q^{-11}(\mathrm{d}/\mathrm{d}q)\ln P$ series. (The introduction of the q^{-11} multiplying factor is explained in IV, §2.) However, the regular alternation in sign suggests that the radius of convergence of (4) is associated with a non-physical singularity on the negative real axis at $q=q^*$ say. This is confirmed by the Dlog Padé approximants which give $q^*\simeq-0\cdot595$. In the complex q-plane a number of complex conjugate pairs of singularities are indicated but their positions are difficult to estimate with any precision.

We plot the poles of the Dlog Padé approximants against the estimates of β, obtained by multiplying the corresponding residues by q_c^{11}, in figure 1. The last few estimates from each of the sequences of $[n+j/n]$ approximants for $j=0, \pm1$ are found to define fairly accurately a single smooth curve. From the figure we estimate

$$\beta=0\cdot42\pm0\cdot005+18\Delta q_c \tag{6}$$

corresponding to $q_c=0\cdot802$. Assuming that $|\Delta q_c|\leq0\cdot003$ as in (5) we obtain the final estimate (3) above.

We have also formed estimates for β from the Padé approximants to $q^{-11}(q-q_c)$ $(\mathrm{d}/\mathrm{d}q)\ln P$ evaluated at $q=q_c$. These are given in table 1. From these and similar results for different values of q_c we conclude that

$$\beta=0\cdot42\pm0\cdot03+20\Delta q_c \tag{7}$$

in good agreement with (6) only with larger uncertainties.

To calculate $P(p)$ numerically we write

$$P(p)=B^*(q)(q_c-q)^{0\cdot42} \tag{8}$$

and evaluate Padé approximants to the series for $(q_c-q)[P(p)]^{-1/0\cdot42}$ in the interval $0\leq q\leq q_c$. Figure 2 is based on the [19/19] approximant but other high-order approximants give identical results to within graphical accuracy. The corresponding plot for the site problem on the triangular lattice (Sykes *et al* 1974) is shown for comparison. The critical amplitude corresponding to the [19/19] approximant is $B^*(0\cdot802)=4\cdot187$.

The limits of uncertainty on our best estimate (3) of β are rather wide; this is because of the slow convergence of the expansion and the presence of several non-physical singularities, especially the dominant one at $q=q^*\simeq-0\cdot595$. In addition, estimates of β are very sensitive to the choice of q_c. The estimate (3) is in good agreement with

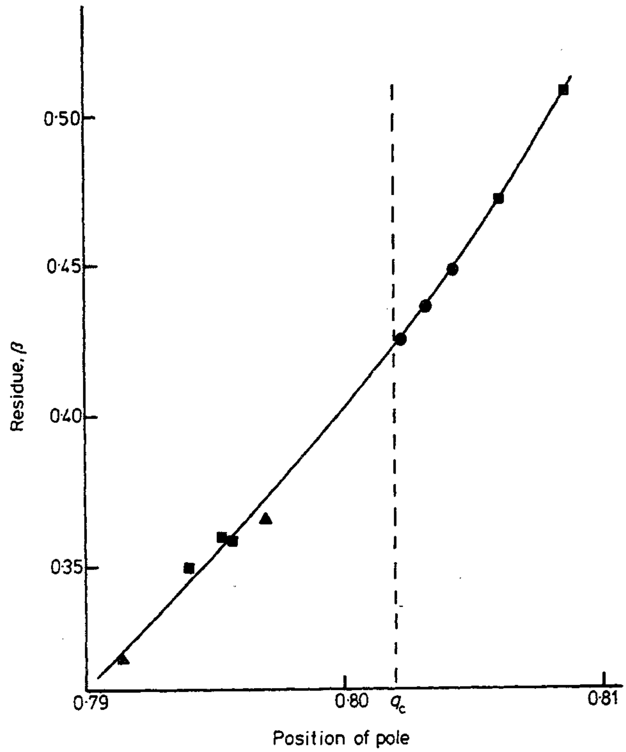

Figure 1. Pole–residue plot for the Dlog Padé approximants to $P(q)$. ▲, $[n-1/n]$; ■, $[n/n]$; ●, $[n+1/n]$.

Table 1. Padé estimates of β from $q^{-11}(q-q_c)(d/dq) \ln P$ with $q_c = 0{\cdot}802$.

n	$[n-1/n]$	$[n/n]$	$[n+1/n]$
10	0·4796	0·4617*	0·4405
11	0·3662	0·6614†	0·4188
12	−0·1752‡	0·4225	0·4167†
13	0·4325	0·4246‡	0·4219*
14	0·4165‡	0·4190‡	0·4201‡
15	0·4281‡	0·4186†‡	0·4218*‡
16	0·4147†‡‡	0·4254*	0·4172†
17	0·4416		

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

evidence from other sources. From the Monte Carlo data of Dean and Bird (1966)†, Kirkpatrick (1973) found that as q_c ranged from 0·798 to 0·802, β ranged from 0·33 to 0·40; the last value corresponds to our estimate of p_c and the estimate for β differs by

† Summarized in Dean and Bird 1967 *Proc. Camb. Phil. Soc.* **63** 477–9.

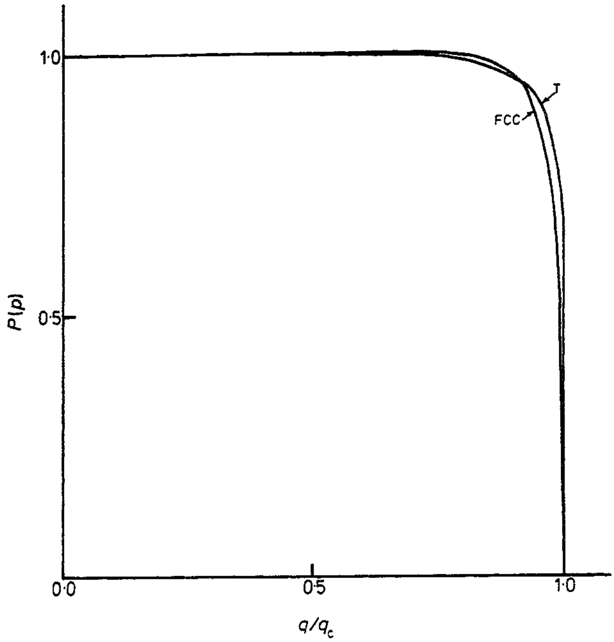

Figure 2. Percolation probability for the site problem on the triangular lattice (T) and the face-centred cubic lattice (FCC) as a function of q/q_c.

only 5%. More recently Kirkpatrick (1976) has obtained $\beta = 0{\cdot}39 \pm 0{\cdot}02$ by graphical analysis of his own Monte Carlo data for the site problem on the simple cubic lattice. The same problem has been studied by Sur *et al* (1976, private communication); by combining their Monte Carlo results for lattices of different size with finite-size scaling theory they obtained $\beta = 0{\cdot}41 \pm 0{\cdot}01$. Assuming ordinary scaling theory to be valid Dunn *et al* (1975) have used their pair connectedness results to predict $\beta = 0{\cdot}39 \pm 0{\cdot}07$. Our final estimate of $\beta = 0{\cdot}42 \pm 0{\cdot}06$ is very close to $5/12 = 0{\cdot}4166\ldots$ which provides a convenient mnemonic.

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