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Percolation exponent δ_p for lattice dimensionality $d \geqslant 3$

David S Gaunt

Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS, UK

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Abstract. Series expansions are used to study the exponent δ_p for site and bond percolation problems on three-dimensional lattices. Our results, which include $\delta_p = 5{\cdot}0 \pm 0{\cdot}8$, are discussed in relation to scaling theory and universality.

To test Toulouse's conjecture regarding the critical dimensionality ($d_c = 6$) for percolation processes, a similar analysis is attempted for the site problem on simple hypercubical lattices of dimensionality $4 \leqslant d \leqslant 7$.

We begin by reporting results obtained from series expansions for the critical exponent δ_p for bond and site percolation processes on various three-dimensional lattices. Our account is brief since the corresponding problem in two dimensions has already been discussed in some detail (Gaunt and Sykes 1976, to be referred to as GS). The basic expansion is given there (GS, equation (1.7)) as

$$P_c(\lambda) = 1 - \sum_{s=1}^{\infty} sD_s(q_c)p_c^{s-1}\lambda^s \tag{1}$$

where the expansion parameter λ is a notional field variable. Estimates of the critical concentration p_c ($= 1 - q_c$) are given by Sykes *et al* (1976a). The number of terms, N, available is limited by the number of perimeter polynomials D_s that are known (Sykes *et al* 1976a). Thus, we have derived expansion (1) through order $N = 7$ FCC(B), 8 BCC(B), 9 SC(B), 13 D(B), 9 FCC(S), 10 BCC(S), 11 SC(S) and 14 D(S). The critical behaviour of $P_c(\lambda)$ (GS, equation (1.8)), assumed to be

$$P_c(\lambda) \sim E_p(1-\lambda)^{1/\delta_p}, \qquad (\lambda \to 1-), \tag{2}$$

has been studied by the standard techniques of series analysis (Gaunt and Guttmann 1974).

According to (2), the expansion coefficients m_n of $-\lambda(d/d\lambda) \ln P_c(\lambda)$ should approach $1/\delta_p$ as $n \to \infty$. Extrapolating adjacent coefficients against $1/n$ gives the linear intercepts which are plotted against n in figure 1. Calculating 'appropriate extrapolants', a smoothing device used in two dimensions, is unnecessary here since the Dlog Padé approximants to $P_c(\lambda)$ show no evidence of disturbing non-physical singularities anywhere in the complex λ-plane. Although the plots are quite smoothly behaved and monotonic, they are very difficult to extrapolate due presumably to confluent correction terms. However, assuming a common limit for bond and site percolation, a value close to $\delta_p = 5$ does not seem unreasonable. Accordingly, we tentatively adopt the estimate

$$\delta_p = 5{\cdot}0 \pm 0{\cdot}8 \tag{3}$$

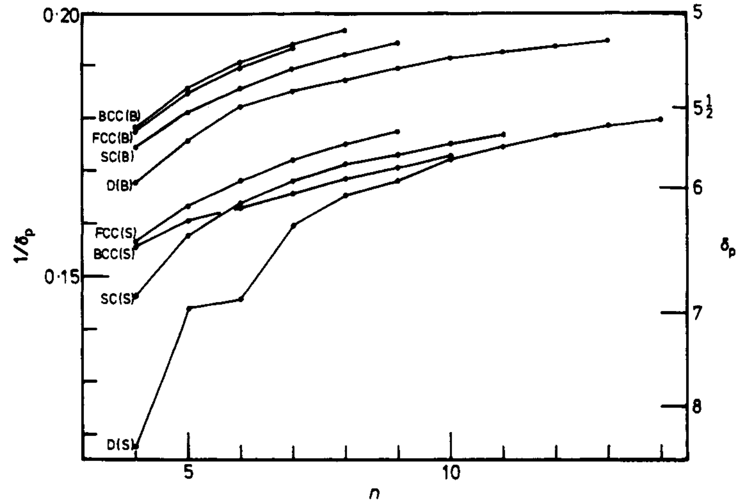

Figure 1. Estimates of $1/\delta_p$ plotted against n for three-dimensional site and bond problems.

where the uncertainty has been chosen to embrace the worst upper bound of $\delta_p < 5{\cdot}8$ for the site problem on the body-centred cubic lattice. A preliminary report of the result (3) has been given elsewhere (Gaunt 1977). The uncertainties in p_c introduce additional uncertainties into (3) of about $\pm 0{\cdot}5$. The apparently anomalous behaviour of the body-centred cubic lattice for both site and bond problems is possibly caused by the uncertainties in p_c.

Alternative but consistent estimates of δ_p are provided by the Padé approximants to the series for $(\lambda-1)(\mathrm{d}/\mathrm{d}\lambda)\ln P_c(\lambda)$ evaluated at $\lambda=1$. The main diagonal $[n/n]$ sequences ($n = 1, 2, \ldots, 6$) for the diamond lattice are:

$$6{\cdot}914, 6{\cdot}916, 5{\cdot}904, 5{\cdot}296, 5{\cdot}474, 5{\cdot}174, \ldots \tag{4}$$

for the bond problem, and

$$7{\cdot}456, 7{\cdot}606, —, 7{\cdot}064, 5{\cdot}523, 5{\cdot}782, \ldots \tag{5}$$

for the site problem. The diamond lattice is chosen since the sequences are longest in this case.

We have estimated the critical amplitude E_p in (2) from the residues at the pole close to $\lambda = 1$ of the Padé approximants to the $P_c^{-\delta_p}$ series, using the central estimate in (3). This method proved the most useful in two dimensions. We find the following estimates for $D_p \equiv E_p^{-\delta_p}$:

$$D_p = \begin{cases} 0{\cdot}25 \pm 0{\cdot}005 \mp 0{\cdot}02 & \text{FCC(B)} \\ 0{\cdot}24 \pm 0{\cdot}02 \ \ \mp 0{\cdot}025 & \text{BCC(B)} \\ 0{\cdot}22 \pm 0{\cdot}015 \mp 0{\cdot}025 & \text{SC(B)} \\ 0{\cdot}20 \pm 0{\cdot}015 \mp 0{\cdot}035 & \text{D(B)} \end{cases} \tag{6}$$

and

$$D_p = \begin{cases} 0{\cdot}21 \pm 0{\cdot}03 \mp 0{\cdot}035 & \text{FCC(S)} \\ 0{\cdot}24 \pm 0{\cdot}02 \mp 0{\cdot}045 & \text{BCC(S)} \\ 0{\cdot}25 \pm 0{\cdot}03 \mp 0{\cdot}045 & \text{SC(S)} \\ 0{\cdot}26 \pm 0{\cdot}03 \mp 0{\cdot}045 & \text{D(S)} \end{cases} \tag{7}$$

where the first uncertainty represents the inherent uncertainty of the method and the second that due to the uncertainties in p_c. Further uncertainties would be introduced by those given in (3) for δ_p. As expected the amplitudes vary monotonically with lattice coordination number for both bond and site problems. Notice, however, that D_p increases with coordination number for the bond problem and decreases for the site problem.

In summary, it appears that our best estimate of $\delta_p = 5{\cdot}0 \pm 0{\cdot}8$ is consistent with δ_p being a dimensional invariant. Earlier work by Essam and Gwilym (1971) based upon shorter series gave the same central result but with much larger uncertainties, namely $1/\delta_p = 0{\cdot}2 \pm 0{\cdot}2$. Exactly the same result is quoted by Stauffer (1975) who re-analysed existing Monte Carlo data.

The direct estimate (3) is in good agreement with

$$\delta_p = 4{\cdot}95^{+0{\cdot}86}_{-0{\cdot}64} \tag{8}$$

obtained using the series estimates (Sykes *et al* 1976a, b)

$$\gamma_p = 1{\cdot}66 \pm 0{\cdot}07, \qquad \beta_p = 0{\cdot}42 \pm 0{\cdot}06, \tag{9}$$

and the scaling law (Essam and Gwilym 1971)

$$\delta_p - 1 = \gamma_p/\beta_p. \tag{10}$$

Other percolation exponents that have been estimated directly include Δ_p and ν_p, the 'constant gap' exponents for the moments of the cluser size distribution and the pair connectedness, respectively. The best scaling predictions, namely

$$\Delta_p = 2{\cdot}08 \pm 0{\cdot}13, \qquad \nu_p = 0{\cdot}83 \pm 0{\cdot}06 \tag{11}$$

are obtained using the numerical estimates (9) and the scaling laws (Essam and Gwilym 1971, Dunn *et al* 1975a)

$$\Delta_p = \beta_p + \gamma_p, \qquad \nu_p = (2\beta_p + \gamma_p)/d, \tag{12}$$

where d is the lattice dimensionality. The predictions (11) are in good agreement with the direct series estimate (Essam *et al* 1976)

$$\Delta_p = 2{\cdot}2 \pm 0{\cdot}1 \tag{13}$$

and (Dunn *et al* 1975b, Cox and Essam 1976)

$$\nu_p = \begin{cases} 0{\cdot}825 + 50\Delta p_c \pm 0{\cdot}02, & \text{FCC(B)} \\ 0{\cdot}83 + 15\Delta p_c \pm 0{\cdot}01, & \text{FCC(S)}. \end{cases} \tag{14}$$

Although the central scaling value of Δ_p is just excluded by the direct estimate, there is a substantial region of overlap when the uncertainties are taken into account.

The numerical estimates in (3), (9), (13) and (14) are quite close to

$$\delta_p = 5, \qquad \gamma_p = 1\tfrac{2}{3}, \qquad \beta_p = \tfrac{5}{12}, \qquad \Delta_p = 2\tfrac{1}{12}, \qquad \nu_p = \tfrac{5}{6}, \tag{15}$$

which we adopt as simple mnemonics that satisfy the scaling laws exactly. In general, the values in (15) lie close to the central direct estimate and certainly well within the quoted uncertainties. The only exception is $\Delta_p = 2\frac{1}{12} = 2{\cdot}0833\ldots$ which lies just outside the range quoted in (13).

Gaunt and Sykes (1976) have speculated as to whether the three-dimensional data would be consistent with δ_p being an even integer, as it seems to be in two dimensions

($\delta_p = 18$) and is for the Bethe lattice ($\delta_p = 2$). Although such a conclusion cannot be ruled out completely, it seems in fact that δ_p is much closer to an odd integer, namely $\delta_p = 5$. As is well known, $\delta = 5$ has been suggested (Gaunt 1967, Gaunt and Sykes 1972) for the three-dimensional Ising model. Although the equality $\delta_p = \delta = 5$ is consistent with 'new' or 'weak' universality (Suzuki 1974), the uncertainty in the numerical estimate of δ_p is really quite large (16%) so that this consistency may well be fortuitous. Certainly weak universality does not appear to hold (GS, § 3) in two dimensions where $\delta = 15$ and the numerical uncertainties in δ_p prohibit any overlap.

A test of universality (or lattice–lattice scaling) for percolation processes can be made by examining the following combination (Betts *et al* 1971) of critical amplitudes:

$$R_p \equiv B_p^{\delta_p - 1} C_p D_p$$

where the amplitudes B_p and C_p correspond to the critical exponents β_p and γ_p, respectively. In two dimensions, it has been demonstrated (Stauffer 1976, Marro 1976) within reasonable bounds that R_p behaves like a universal quantity for both bond and site problems. For three-dimensional lattices, the amplitudes D_p are given in (6) and (7), and the C_p are given by Sykes *et al* (1976a). For B_p, slow convergence of the series prevented Sykes *et al* (1976b) from drawing any firm conclusions except for the face-centred cubic site problem for which a rough estimate was quoted without uncertainties. If the uncertainty in B_p does not exceed 4%—in two dimensions it is less than 1%—then $R_p \simeq 6{\cdot}5 \pm 3$. Assuming R_p to be universal for three-dimensional site problems, yields the following predictions for B_p:

$$3{\cdot}7 \pm 0{\cdot}7 \quad \text{BCC(S)}, \qquad 3{\cdot}4 \pm 0{\cdot}7 \quad \text{SC(S)}, \qquad 3{\cdot}1 \pm 0{\cdot}6 \quad \text{D(S)}. \tag{16}$$

If the same value of R_p also obtains for bond problems, then we find for B_p:

$$\begin{array}{llll} 5{\cdot}0 \pm 0{\cdot}8 & \text{FCC(B)}, & 4{\cdot}4 \pm 0{\cdot}7 & \text{BCC(B)}, \\ 3{\cdot}95 \pm 0{\cdot}65 & \text{SC(B)}, & 3{\cdot}5 \pm 0{\cdot}7 & \text{D(B)}. \end{array} \tag{17}$$

Finally, let us consider the way in which $\delta_p(d)$ approaches its Bethe value ($\delta_p = 2$) as the dimensionality d approaches the critical dimension d_c. It has been conjectured (Toulouse 1974) that d_c for percolation is $d_c = 6$ rather than $d_c = 4$ as found for second-order phase transitions with short-range interactions. This has been tested numerically by Gaunt *et al* (1976), who derived series for the mean cluster size of site mixtures on a d-dimensional simple hypercubical lattice and estimated $\gamma_p(d)$ for $d \leqslant 6$. Their results, which were in broad agreement with the Monte Carlo estimates of Kirkpatrick (1976), supported Toulouse's hypothesis to within the accuracy attainable. Analysis of the closely related cluster growth problem indicates $d_c = 6$ in this case also (Gaunt *et al* 1976). In the present work, we have used the first seven perimeter polynomials given by Gaunt *et al* (1976) *for general d* to derive $P_c(\lambda)$ through λ^7 for $d = 4, 5, 6$ and 7. Numerical estimates of $p_c(d)$ are given in table 3 of Gaunt *et al* (1976), except for $d = 7$ where we have used $p_c(7) = 0{\cdot}089 \pm 0{\cdot}003$ (Gaunt, unpublished work). The series have been analysed by the method employed to plot figure 1 of the present paper. The results are exhibited in figure 2. For $d = 3$, the curve is that already given in figure 1 for the simple cubic site problem. The $d = 2$ plot is for the simple quadratic site problem and is taken from figure 1 of GS, where it continues up to $n = 17$. The uncertainties produced by uncertainties in p_c are between 10 and 15%, except for $d = 2$

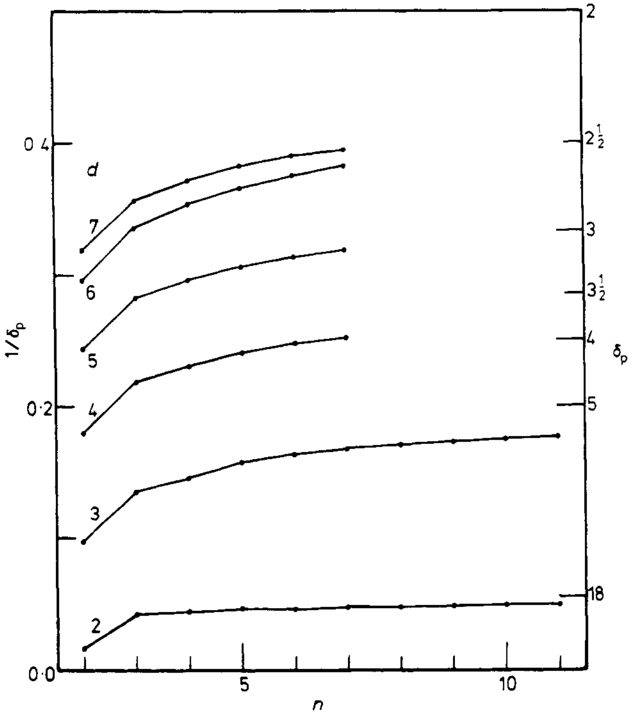

Figure 2. Estimates of $1/\delta_p$ plotted against n for the site problem on simple hypercubical lattices of dimensionality $d = 2, 3, \ldots, 7$.

where they are only 4%. Although the curves are not easily extrapolable, we draw two tentative conclusions. First, it is not difficult to accept the possibility of a common limit for $d = 6$ and 7 (presumably $\delta_p = 2$). Second, while not excluding the possibility, the evidence seems rather against $\delta_p(4) = 4$ and $\delta_p(5) = 3$, in which case δ_p cannot be integer in all dimensions.

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