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COMMENT

On the percolation threshold for a *d*-dimensional simple hypercubic lattice

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Abstract. We use $1/\sigma$-expansions ($\sigma = 2d-1$) to investigate systematically a number of conjectures and approximations for the bond and site percolation thresholds of a d-dimensional simple hypercubic lattice. The technique provides convincing evidence that none of the conjectures are correct and gives a quantitative understanding of the quality of the approximations.

Bond and/or site percolation thresholds p_c have been calculated *rigorously* (Kesten 1980, 1982, Wierman 1981) for some two-dimensional planar lattices and *conjectured* (e.g. Tsallis 1982) for several others. The critical exponents for percolation in $d=2$ dimensions have been *conjectured* by den Nijs (1979), Pearson (1980) and Nienhuis *et al* (1980) and are supported by a considerable body of numerical and theoretical evidence. They are widely believed to be exact, the evidence being conveniently summarised in the review by Sahimi (1983).

Recently, a number of workers, encouraged perhaps by the apparent success of the above conjectures, have tried to conjecture the exact percolation threshold for lattices with $d \geqslant 3$. In this comment we propose a simple method for checking such conjectures and find compelling evidence that *none of them are exact.* In addition, the method enables us to understand in a quantitative way why sometimes the approximation is rather good even though the conjecture is not correct. The technique involves expanding the conjectured expression for p_c in inverse powers of σ where $\sigma = q-1$. (For a simple hypercubic lattice, the coordination number $q = 2d$.) This expansion may then be compared with either the expansion of Gaunt *et al* (1976) for site percolation,

$$p_c^{(S)} = \sigma^{-1} + 1\tfrac{1}{2}\,\sigma^{-2} + 3\tfrac{3}{4}\,\sigma^{-3} + 20\tfrac{3}{4}\,\sigma^{-4} + \ldots, \tag{1}$$

or that of Gaunt and Ruskin (1978) for bond percolation

$$p_c^{(B)} = \sigma^{-1} + 2\tfrac{1}{2}\,\sigma^{-3} + 7\tfrac{1}{2}\,\sigma^{-4} + 57\,\sigma^{-5} + \ldots. \tag{2}$$

These results are expected to coincide with the exact $1/\sigma$-expansions for p_c—assuming their existence—since their derivation, although not rigorous, is formally exact. (Rigorous evidence for the existence of $1/\sigma$-expansions exists for the spherical model (Gerber and Fisher 1974), the self-avoiding walk problem (Kesten 1964) and for directed bond percolation (Cox and Durret 1983).) As expected, the first-order term in (1) and (2) gives the correct limiting ($d \to \infty$) behaviour as given by the Bethe approximation. The expansions are probably asymptotic, although it is only for the

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spherical model that the analogous statement has been proven rigorously (Gerber and Fisher 1974).

The basic idea of comparing $1/\sigma$-expansions is not new. It has been used both for demonstrating likely *equality* (Whittington *et al* 1983, Gaunt *et al* 1984) and for suggesting strict *inequalities* (Gaunt and Ruskin 1978, Gaunt *et al* 1982, 1984) between various critical points arising in the study of percolation, self-avoiding and neighbour-avoiding walks, lattice trees, lattice trees with specified topologies, unrestricted lattice animals and lattice animals with a prescribed number of cycles. Harris (1983) has used the idea to demonstrate the falsity of a conjecture concerning $p_c^{(B)}(d)$ due to Sahimi *et al* (1983) and here we apply it to the investigation of a range of conjectures and approximations to p_c (denoted by $\hat{p}_c$).

We begin by considering the conjecture of Sahimi *et al* (1983) and make a number of points not considered in the analysis of Harris (1983). Explicitly, Sahimi *et al* conjecture, on the basis of numerical evidence, that

$$\hat{p}_c^{(B)} = G_0 \tag{3}$$

may be exact for three- and higher-dimensional Bravais lattices. The quantity G_0 is a lattice Green function important in the theory of random lattice walks. From the work of Montroll (1956), it follows that (3) may be written as

$$\hat{p}_c^{(B)} = G_0 = q^{-1}(1-f)^{-1} = q^{-1}F \tag{4}$$

where $f = 1 - F^{-1}$ is the probability of eventual return to the origin. Asymptotic expansions in inverse powers of q for both f and F are given by Montroll† through $O(q^{-5})$. Substituting either of these expansions into (4) and then re-expanding in powers of $1/\sigma$ gives

$$\hat{p}_c^{(B)} = \sigma^{-1} + 2\sigma^{-3} + 5\sigma^{-4} + 27\sigma^{-5} + 149\sigma^{-6} + \ldots. \tag{5}$$

This result should be compared with the presumably exact expansion given in (2). The first-order term in (5) gives the correct limiting behaviour; also (5) has no σ^{-2} term in agreement with (2). However, differences in the magnitudes of the coefficients appear at $O(\sigma^{-3})$ and increase with the order of the term. We find

$$p_c^{(B)} - \hat{p}_c^{(B)} = \tfrac{1}{2}\sigma^{-3} + 2\tfrac{1}{2}\sigma^{-4} + 30\sigma^{-5} + \ldots. \tag{6}$$

Clearly the conjecture (3) *of Sahimi et al can only be an approximation.* This conclusion was also reached by Harris (1983) who derived the leading term in (6) and also by Wilke (1983). Wilke simply compared his rather precise Monte Carlo estimate of $p_c^{(B)} = 0.2492 \pm 0.0002$ for the simple cubic lattice with the conjectured value of $G_0 = 0.252\,731\ldots$ (Montroll 1956). The expansion (6) *suggests* (but does not prove) that $p_c^{(B)} > G_0$ *for sufficiently large d.* Evidently the inequality just fails for $d = 3$, while for $d = 2$ it is clearly violated since $p_c^{(B)} = \frac{1}{2}$ and G_0 is infinite. However, the inequality appears to be satisfied for $d = 4$, 5, 6 and 7 (and presumably larger d) by the series estimates of p_c tabulated by Gaunt and Ruskin (1978).

In view of the above remarks it is most unlikely that the conjecture (3) is exact for any of the other three-dimensional Bravais lattices considered by Sahimi *et al* (1983).

The following question was raised by Sahimi *et al*: if the conjecture is not correct, why does the approximation appear to be so good? From (6) and (2), one sees that

† There is an error in the expansion for F. The last coefficient quoted should read $10(71)/2q^5$.

for large d the relative percentage error $(p_c^{(B)} - \hat{p}_c^{(B)})/p_c^{(B)} \approx 50\sigma^{-2}$. At the upper critical dimension $d_{c,u} = 6$, this has decreased to about 0.4% which is comparable to the uncertainty in the best numerical estimate of $p_c^{(B)}$ (Gaunt and Ruskin 1978).

We turn our attention now to two older approximations. The single-bond effective medium approximation (Kirkpatrick 1973) provides physical motivation for the formula

$$\hat{p}_c^B = 2/q. \qquad (7)$$

Expanding in powers of $1/\sigma$ gives the (convergent) expansion

$$\hat{p}_c^{(B)} = 2\sigma^{-1} - 2\sigma^{-2} + 2\sigma^{-3} - 2\sigma^{-4} + \dots, \qquad (8)$$

the leading term of which does not even give the correct limiting $(d \to \infty)$ behaviour.

An empirical formula due to Vyssotsky *et al* (1961),

$$\hat{p}_c^{(B)} = d(d-1)^{-1}q^{-1}, \qquad (9)$$

which reduces to (7) when $d = 2$, takes the form

$$\hat{p}_c^{(B)} = \tfrac{1}{2}(d-1)^{-1} \qquad (10)$$

for a d-dimensional simple hypercubic lattice. This form of the approximation has also been discussed more recently by Kirkpatrick (1979) and by Chao (1982). From (10) we obtain the (convergent) expansion

$$\hat{p}_c^{(B)} = \sigma^{-1} + \sigma^{-2} + \sigma^{-3} + \sigma^{-4} + \dots \qquad (11)$$

which has the correct dominant behaviour but whose leading correction term is of the wrong order.

Besides their simplicity the main advantage of approximations such as (7) and (10) seems to be the fact that they give good results for *small d*. For example, (7) gives the exact results for $d = 1$ and the $d = 2$ square lattice, while (10) is exact for $d = 2$ and provides a rather good approximation for $d = 3$ (Wilke 1983).

Very recent work, which also gives good results for small d, is due to Hajdukovic (1983). This approximation gives an explicit expression for the critical point $K_c(d, s)$ of the s-state Potts model on a simple hypercubic lattice for arbitrary d. For the bond percolation $(s \to 1)$ problem (Kasteleyn and Fortuin 1969, Wu 1978), the conjecture is

$$\hat{p}_c^{(B)} = 1 - e^{-\hat{K}_c(d,1)} = 1 - 2^{-2/d(d-1)}. \qquad (12)$$

For $d = 1$ and 2 this yields the exact results but, as pointed out by Wu (1984), the prediction of $\hat{p}_c^{(B)} = 1 - 2^{-1/3} = 0.206\,299\dots$ for the simple cubic lattice $(d = 3)$ differs appreciably from the best numerical estimates. The validity of the conjecture for general s and d is, therefore, clearly suspect. To confirm this suspicion we simply expand (12) giving

$$\hat{p}_c^{(B)} = a\sigma^{-2} + a(1 - \tfrac{1}{2}a)\sigma^{-4} + a(1 - a + \tfrac{1}{6}a^2)\sigma^{-6} + \dots, \qquad (a = 8 \ln 2), \qquad (13)$$

whereupon comparison with (2) shows that not even the dominant $(d \to \infty)$ behaviour is given correctly. Indeed it appears to have escaped prior notice that the conjectured value (12) violates the rigorous inequality $p_c^{(B)} \geq \sigma^{-1}$ for $d \geq 4$. (The inequality follows by combining the rigorous inequality $p_c^{(B)} \geq \mu^{-1}$ (Broadbent and Hammersley 1957) with the rigorous but trivial inequality $\mu \leq q - 1 = \sigma$ for the self-avoiding walk limit μ.)

So far, all of the approximations we have discussed have been for the bond percolation threshold. The only analogous expression known to us for site percolation is the empirical formula

$$\hat{p}_c^{(S)} = d(2d-1)^{-1}(d-1)^{-1} \tag{14}$$

for simple hypercubic lattices with $d \geqslant 3$ due to Sahimi *et al* (1983). Expanding in $1/\sigma$ gives the (convergent) expansion

$$\hat{p}_c^{(S)} = \sigma^{-1} + 2\sigma^{-2} + 2\sigma^{-3} + 2\sigma^{-4} + \ldots. \tag{15}$$

Comparison with (1) shows that the dominant behaviour is given correctly, as is the order of the leading correction term—but not its magnitude. For the relative percentage error we find using (1) and (15) that $(\hat{p}_c^{(S)} - p_c^{(S)})/p_c^{(S)} \approx 50\sigma^{-1}$ for large d. This is much worse than $50\sigma^{-2}$ resulting from the approximation of Sahimi *et al* and which (as seen earlier) is the best large d result for bond percolation.

To summarise, we have used $1/\sigma$-expansions to investigate a number of conjectures and approximations for the bond and site percolation thresholds of d-dimensional simple hypercubic lattices. The technique demonstrates quite convincingly that none of the conjectures are exact and gives a clear and quantitative understanding as regards the quality of the approximations. Clearly it is not limited to the percolation problem but may be applied to any of the problems for which $1/\sigma$-expansions are available. In all cases, we strongly recommend the early application of this technique to the examination of potential conjectures and the assessment of likely approximations.

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