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LETTER TO THE EDITOR

On Pólya random walks, lattice Green functions, and the bond percolation threshold

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Abstract. Based on numerical evidence, we conjecture a connection between the bond percolation threshold of Bravais lattices in three or more dimensions and the value at the origin of a lattice Green function related to the probability of return to the origin for a Pólya random walk.

Percolation theory has become a powerful, much-used tool of physics. Its popularity stems from its potential applications to a variety of fields, and from the fact that despite the simplicity of its underlying concepts, it leads to non-trivial critical phenomena. (For recent reviews see Essam (1980) and Stauffer (1979).) Despite extensive study, few exact results have been obtained for the most interesting quantities in percolation theory. In particular, the catalogue of exact results concerning the bond and site percolation thresholds p_c^B and p_c^S has few entries. For the one-dimensional lattice (the linear chain) it is known trivially that $p_c^B = p_c^S = 1$, while for a Bethe lattice (Cayley tree) of coordination number z, Fisher and Essam (1961) have shown that $p_c^B = p_c^S = 1/(z-1)$. (Fisher and Essam have also derived exact thresholds for some other pseudolattices related to the Bethe lattice.) By a not entirely rigorous argument, Sykes and Essam (1964) derived the bond percolation thresholds p_c^B for three two-dimensional lattices: hexagonal, $1-2\sin(\pi/18)$; triangular, $2\sin(\pi/18)$; square, $1/2$. Their arguments have subsequently been made completely rigorous by Kesten (1980) and Wierman (1981). Sykes and Essam also give two exact site percolation thresholds: triangular, $1/2$; Kagomé, $1-2\sin\pi/18$.

The work of Kasteleyn and Fortuin (1969) and Fortuin and Kasteleyn (1972) establishes that the bond percolation problem is the $q \to 1$ limit of the q-state Potts model; a simpler derivation of this result has been given by Wu (1978). It is therefore not surprising that exact results on p_c^S and p_c^B, and presumably exact results on critical exponents for percolation properties (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980), are available only for the linear chain, the Bethe lattice and two-dimensional lattices. A few rigorous inequalities involving p_c^S and p_c^B are available. One of these relates percolation processes to *self-avoiding walks*:

$$p_c^S \geqslant p_c^B \geqslant 1/\mu \tag{1}$$

(Broadbent and Hammersley 1957). Here $\mu = e^{\kappa}$ denotes the connective constant of the lattice, and if C_n is the number of self-avoiding walks of n steps, $\kappa = \lim_{n\to\infty}(1/n)\ln C_n$ (Hammersley 1957a). For a lattice with coordination number z at

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each site, $\mu \leqslant z-1$, so that equation (1) implies the simpler, but weaker, inequality

$$p_c^S \geqslant p_c^B \geqslant 1/(z-1); \tag{2}$$

apart from the Bethe lattice the inequalities are believed to be strict.

Numerical values of p_c^S and p_c^B can be determined by a variety of means, the degree of precision being of course limited by constraints of computational cost. Some estimates of p_c^B are collected in tables 1 and 2, as discussed below. Both physically motivated and empirical approximate formulae are available. A single-bond effective medium approximation (Kirkpatrick 1973) gives

$$p_c^B = 2/z \tag{3}$$

for a lattice of coordination number z, irrespective of dimension. In two dimensions, this approximation is excellent, being exact for the square lattice and in small error for the triangular and hexagonal lattices. By refining the effective medium approach, Turban (1978) has reproduced the known exact values of p_c^B for the triangular and hexagonal lattices. Accurate approximations in dimensions higher than two are harder to obtain. Vyssotsky *et al* (1961) note in particular that

$$p_c^B \simeq d/(d-1)z \tag{4}$$

(with d the dimension) is excellent for $d=2$ and fairly good for $d=3$. Any approximation for p_c^B must be consistent with the limiting behaviour

$$p_c^B \geqslant 1/(z-1), \qquad p_c^B \sim 1/(z-1) \qquad \text{as } d \to \infty. \tag{5}$$

Recently, the authors noticed that a certain quantity gives values very close to the numerical predictions of p_c^B for Bravais lattices in three or more dimensions. With $\{i\}$ denoting the set of nearest neighbours of site i, a lattice Green function G_i can be defined as the unique solution of the equation (Sahimi *et al* 1982)

$$zG_i - \sum_{j \in \{i\}} G_j = \delta_{i0} \tag{6}$$

which decays to zero as the distance of site i from the origin increases. (Such a solution exists only in three or higher dimensions.) Our observation is that

$$p_c^B \simeq G_0 \tag{7}$$

in three or more dimensions. We conjecture that this result may in fact be exact, based on numerical evidence discussed below. The quantity G_0 can frequently be found from Fourier analysis. In particular, if sites of the lattice can be mapped onto a d-dimensional sublattice of the d-dimensional hypercubic lattice $\mathbb{Z}^d$ then

$$G_0 = \frac{1}{(2\pi)^d z} \int_{-\pi}^{\pi} \cdots \int \frac{\mathrm{d}^d \boldsymbol{\theta}}{1-\lambda(\boldsymbol{\theta})}, \tag{8}$$

where

$$\lambda(\boldsymbol{\theta}) = z^{-1} \sum_{l \in \{0\}} \mathrm{e}^{\mathrm{i}\boldsymbol{\theta}\cdot\boldsymbol{l}} \tag{9}$$

is the structure function of the lattice. Integrals of the form (8) figure prominently in the theory of lattice random walks (Montroll 1956). In particular,

$$R = 1 - \{zG_0\}^{-1} \tag{10}$$

is the probability of eventual return to the origin of a Pólya (unbiased, nearest-neighbour stepping) random walk. Thus, the expression (7) is equivalent to

$$p_c^B \simeq 1/z(1-R). \tag{11}$$

Since $R > 1/z$ and $R \to 1/z$ from above with increasing dimension, the right-hand side of (11) has the correct limiting behaviour (5) as $d \to \infty$.

In table 1, we collect various numerical evaluations and approximations for p_c^B for three-dimensional Bravais lattices. It can be seen from this table that the approximation $p_c^B \simeq G_0$ is excellent and far superior to the effective medium approximation (3) and the empirical formula (4). In table 2, we examine the performance of the various approximations for simple cubic lattices of dimension d, with $3 \leq d \leq 7$. The approximation $p_c^B \simeq G_0$ is again excellent. In general, our expression for p_c^B agrees best with numerical values derived from series expansions. We point out that the stated errors for numerical values of p_c^B represent the degree of confidence in the values, not rigorous bounds on the values.

Table 1. Approximations to the bond percolation threshold p_c^B for three-dimensional Bravais lattices. The sources for the numerical estimates are: [a] Sykes *et al* (1976), [b] Vyssotsky *et al* (1961), [c] Kirkpatrick (1979, p 339), [d] Nakanishi and Stanley (1981), [e] Dunn *et al* (1975), [f] Cox and Essam (1976), via pair-connectedness. It has been shown by Ishioka and Koiwa (1978) that the probability of return to the origin for a Pólya random walker is the same for the face-centred cubic and hexagonal close-packed lattices.

Lattice	Analytic approximations EMA $(2/z)$	$d/[(d-1)z]$	G_0	Numerical estimates Series expansions	Monte Carlo
Simple cubic	0.333 33	0.250 00	0.252 73	0.247 ± 0.003[a]	0.2495 ± 0.0005[c] 0.254 ± 0.013[b] $0.25 \pm ?$[d]
Body-centred cubic	0.250 00	0.187 50	0.174 15	0.1785 ± 0.002[a]	—
Face-centred cubic	0.166 67	0.125 00	0.112 06	0.119 ± 0.001[a] 0.119 ± 0.0005[e] $0.1185 \pm ?$[f]	0.125 ± 0.005[b]
Hexagonal close-packed	0.166 67	0.125 00	0.112 06	—	0.124 ± 0.005[b]

Table 2. Approximation to the bond percolation threshold p_c^B for d-dimensional simple cubic lattices. The numerical estimates are from [a] combination of all sources in table 1; [b] Gaunt and Ruskin (1978); [c] Kirkpatrick (1979, p 339). For $d \geq 4$, G_0 is evaluated using (8) and the asymptotic expansion for R derived by Montroll (1956).

d	$1/(z-1)$	$d/[(d-1)z]$	G_0	Numerical estimates
3	0.2000	0.250	0.252 73	$0.25 \pm ?$[a]
4	0.1429	0.1667	0.156	0.161 ± 0.0015 0.1435 ± 0.001[c]
5	0.1111	0.1250	0.115	0.118 ± 0.001
6	0.0909	0.1000	0.093	0.094 ± 0.0005
7	0.0769	0.0833	0.078	0.078 ± 0.0002

We have no theoretical argument to support the conjecture that $p_c^B = G_0$ for $d \geqslant 3$, or to explain, if the conjecture is not correct, why the approximation is so good. However, since the lattice Green function G_i contains information on the topological structure of the lattice, the possibility that it is related in some manner to quantities of percolation theory might be anticipated. The relation $p_c^B = G_0$ is not here conjectured to hold for arbitrary periodic lattices, but only for Bravais lattices in three or more dimensions. For the diamond lattice, which is not a Bravais lattice, $G_0 \simeq 0.44822$ (Ishioka and Koiwa 1978), while numerical determinations of p_c^B by Sykes *et al* (1976) and Vyssotsky *et al* (1961) yield the values 0.388 ± 0.005 and 0.390 ± 0.011 respectively.

An attempt to relate *site percolation thresholds* p_c^S to random walk statistics has been made by Ishioka and Koiwa (1978). They observe from numerical evidence that for periodic lattices of dimension greater than 3,

$$p_c^S \leqslant R; \tag{12}$$

equality in this expression holds for the Bethe lattice (Hughes and Sahimi 1982). However, the heuristic argument Ishioka and Koiwa present in support of (12), based on the mean number S_n of distinct sites visited in an n-step Pólya walk having the asymptotic behaviour $S_n \sim n/\{zG_0\}$, is not entirely convincing. The Ishioka–Koiwa inequality (12) and our expression (11) suggest that the possible connections of percolation theory to *Markovian random walks* may prove more fruitful than better-known connections to *self-avoiding walks*. Further support for this is provided by work of Mauldon (1961), Wu and Stanley (1982) and Reich and Leath (1978). By treating the percolation problem as a Markov process, Mauldon obtained a very strong lower bound for the bond percolation threshold of a fully directed square lattice. His result ($p_c^B \geqslant 0.6297$) compares very well with the value $p_c^B = 0.643 \pm 0.002$ found by Blease (1977) using series expansions. In contrast, Hammersley (1975b) used the better known (non-Markovian) self-avoiding walk connection, obtaining the much weaker lower bound of 0.59697. Wu and Stanley established an exact correspondence between Markovian random walks and a class of directed percolation problems. Reich and Leath studied high-density percolation on a Bethe lattice, i.e. a percolation problem in which only those occupied sites which have at least m nearest-neighbour sites occupied are considered active. They derived the percolation threshold for such a system for arbitrary m using a Markov random walk argument.

There is a curious connection between our result (7) and the spherical model. Let $T_c(q)$ denote the dimensionless critical temperature of the q-state Potts model. Then the Fortuin–Kasteleyn relation (Wu 1978) links p_c^B to $T_c(1+) = \lim_{q \to 1} T_c(q)$:

$$p_c^B = 1 - \exp(-1/T_c(1+)). \tag{13}$$

Equation (7) therefore leads to an expression for $T_c(1+)$ in terms of G_0. On the other hand, the spherical approximation (Berlin and Kac 1952, Joyce 1972) applied to the two-state Potts model, i.e. the Ising model, gives $T_c(2) \simeq (zG_0)^{-1}$, where z is the coordination number of the lattice. This approximation is useful only in three or more dimensions, and improves with increasing z; however, it does establish an approximate relation between $T_c(2)$ and G_0. The interesting possibility arises that an approximation in terms of G_0 might be able to be found for $T_c(q)$ for general q in three or more dimensions.

We have found no expression analogous to (7) for the site percolation threshold. However, we note that the empirical formula

$$p_c^S \simeq d/(2d-1)(d-1) \tag{14}$$

is very good for simple cubic lattices of dimension $d \geqslant 3$, the greatest error being about three per cent at $d = 3$,

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