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LETTER TO THE EDITOR

New approach to percolation: lattice system results

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Abstract. Results of an integral-equation approach to pair connectedness are given for lattice models, with emphasis on site percolation. The lowest-order approximation is expressible in terms of the lattice Green function and is isomorphic to a Pólya random walk. It yields percolation exponents $\gamma=2$, $\nu=1$ for $d=3$ and $\gamma=1$, $\nu=\frac{1}{2}$ for $d\geqslant 4$, $d=$dimension. For simple hypercubic lattices it also yields usefully sharp estimates for the site percolation threshold probability p_P. A first correction is described.

This work is part of a more general investigation of clustering and connectivity we have been making that encompasses percolation and gelation (Ziff and Stell 1980, Ziff *et al* 1984, Chiew *et al* 1985, Klein and Stell 1985) and molecular and ionic association (Høye and Olaussen 1980a, b, 1981, Cummings and Stell 1983, 1984). The results herein are based on an integral-equation approach to pair connectedness that one of us (Stell 1984) recently introduced to permit a general treatment of connectivity in lattice and continuum models. Here we apply that approach to lattice models, with emphasis on site percolation in simple hypercubic lattices. Our lowest-order result, which is of Ornstein–Zernike (OZ) form, proves to be directly expressible in terms of lattice Green functions. The critical exponents we have evaluated in this approximation are $\gamma=2$, $\nu=1$ for $d=3$ and $\gamma=1$, $\nu=\frac{1}{2}$ for $d\geqslant 4$, $d=$dimensionality. For the classic site percolation (SP) problem, the approximation is exact for $d=1$ and exact for the Bethe lattice. On simple hypercubic lattices it yields a particularly useful estimate for p_P, the occupation probability at the percolation point. Our result for p_P is illuminated by an isomorphism we establish between the approximation and a Pólya random walk, which yields for the standard SP problem the relation $p_P=R$, where R is the return probability of the walk. We give also an expression for the first-order correction to our results appropriate to both the standard SP problem and a randomly centred hypercube problem.

Our general approximation scheme is applicable to any lattice but our explicit concern here will be the d-dimensional cubic lattice with unit spacing between nearest-neighbour sites such that

(a) the sites are occupied randomly by particles with mean number density ρ. Two adjacent sites are considered connected if each is occupied by one or more particles, yielding a randomly centred hypercubic (RCH) model, or

(b) an additional constraint of no multiple occupancy of sites is further imposed, yielding the classic site-percolation (SP) model.

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In considering lattice models, the pair connectedness function $\rho^2 h^+(\boldsymbol{r}_{12})$ introduced by Coniglio *et al* (1977) and used in Coniglio and Essam (1977), De'Bell and Essam (1981) and Stell (1984) reduces to the lattice pair connectedness function earlier introduced by Essam (1973). Here $\rho^2 h^+(\boldsymbol{r}_{12})\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2$ is the probability of finding a particle in the volume element $\mathrm{d}\boldsymbol{r}_1$ and another particle in the element $\mathrm{d}\boldsymbol{r}_2$ with both particles joined by at least one path over connected sites. On a lattice $\mathrm{d}\boldsymbol{r}_i$ is taken to be the volume Ω of the Wigner-Seitz cell associated with the ith site. (We assume $\Omega = 1$ unless otherwise noted.) We introduce here the pair connectedness direct correlation function via the Ornstein-Zernike (OZ) equation, which for a lattice can be written in real space as

$$h^+(\boldsymbol{r}_{12}) = c^+(\boldsymbol{r}_{12}) + \rho \sum_i h^+(\boldsymbol{r}_{1i}) c^+(\boldsymbol{r}_{i2}) \tag{1}$$

and in Fourier space as

$$\tilde{h}^+(\boldsymbol{k}) = \tilde{c}^+(\boldsymbol{k})[1 - \rho \tilde{c}^+(\boldsymbol{k})]^{-1} \tag{2}$$

where, for a function $a(r)$,

$$\tilde{a}(\boldsymbol{k}) = \sum_j a(\boldsymbol{r}_j) \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}_j). \tag{3}$$

In the series-union/Percus-Yevick (SU/PY) approximation considered by Stell (1984),

$$c^+(\boldsymbol{r}) = 0 \qquad \text{for } \boldsymbol{r} > 1 \tag{4}$$

in both our models. Let

$$c^+(\boldsymbol{r}) = c_0 \qquad \text{for } r = 0, \qquad c^+(\boldsymbol{r}) = c_1 \qquad \text{for } r = 1,\ r = |\boldsymbol{r}|. \tag{5}$$

Then for simple cubic lattices

$$\tilde{c}^+(\boldsymbol{k}) = c_0 + 2c_1 \sum_{i=1}^{d} \cos k_i \tag{6}$$

where k_i are the cartesian components of $\boldsymbol{k}$. We introduce in corresponding notation

$$h^+(\boldsymbol{r}) = h_0 \qquad \text{for } r = 0, \qquad h^+(\boldsymbol{r}) = h_1 \qquad \text{for } r = 1. \tag{7}$$

Then in the SP model

$$h_0 = 0, \qquad h_1 = 1, \tag{8}$$

and in the RCH model

$$h_0 = h_1 = 1. \tag{9}$$

We note that in both models (as in the continuum randomly centred sphere model considered by Chiew and Glandt (1983), and by Stell (1984)) the SU/PY approximation can equally well be regarded as a mean spherical (MS) approximation, with $c^+(\boldsymbol{r}) = 0$ outside a core region in which $h^+(\boldsymbol{r})$ is explicitly prescribed by an occupancy constraint.

Let K^2 be the ratio of the zeroth spatial moment of $\delta_{r,0} + \rho h(\boldsymbol{r})$ to its second moment and z the lattice coordination number. Then $z^{-1/2}K = \kappa$ is an inverse correlation length that becomes zero at the percolation point, with $1 + K^2 = (1 - \rho c_0)/z\rho c_1$. In both models, we find

$$\delta_{r,0} + \rho h^+(\boldsymbol{r}) = G(K, \boldsymbol{r})/\rho c_1 \tag{10}$$

where $G(K, \boldsymbol{r})$ is the lattice Green function for the lattice Helmholtz equation and

$G(0, \boldsymbol{r})$ the lattice Green function for the lattice Poisson equation. For simple cubic lattices

$$zG(K, \boldsymbol{r}) = \frac{\Omega}{(2\pi)^d} \int_{\mathrm{BZ}} \frac{\cos \boldsymbol{r}\cdot\boldsymbol{k}\,\mathrm{d}\boldsymbol{k}}{(K^2+1) - z^{-1}\,\Sigma_j \cos k_j}, \qquad 1 \leqslant j \leqslant z.$$

In earlier work, Stell (1969) obtained the basic relation

$$zG(K, 0) = I(1 + \mathrm{constant}_1\, K^2 + \mathrm{constant}_2\, K^{d-2} + \mathrm{constant}_3\, K^{d-2} \ln K + \ldots). \tag{11}$$

Here I is a Watson integral, the $\mathrm{constant}_1$ and $\mathrm{constant}_2$ are non-zero, and $\mathrm{constant}_3 = 0$ when and only when d is odd. The ellipsis in (11) represents terms that are always dominated by at least one of the exhibited terms. Letting

$$G(K, \boldsymbol{r}) = G_0 \quad \text{at } r = 0 \quad \text{and} \quad G_1 \text{ at } r = 1 \tag{12}$$

we can relate G_0 and G_1 through a Green function identity. For the simple cubic lattice

$$zG_1 = (K^2+1)zG_0 - 1. \tag{13}$$

From (10), this further yields

$$\rho h_1/(1+\rho h_0) = [(K^2+1)zG_0 - 1]/zG_0. \tag{14}$$

From this we find at the percolation point $K = 0$ in the SP case, using (8) and (11), $\rho = (I-1)/I$. So the percolation density ρ_{P} (equivalently, the site occupancy probability p_{P}) is given by

$$\rho = p_{\mathrm{P}} = (I-1)/I. \tag{15}$$

Following the method of Stell (1969) (see also appendix of Stell 1975) we can immediately read off certain critical exponents. At ρ_{P}, from (10) we find that the spatial decay of $h^+(\boldsymbol{r})$ for $r \to \infty$ is like constant $\times\, r^{-d+2-\eta}$ with $\eta = 0$ while from (8), (10) and (11) we see that

$$\rho = \rho_P - \Delta\rho = I^{-1}[(I-1) + \mathrm{constant}\ K^2 + \mathrm{constant}\ K^{d-2} + \mathrm{constant}\ K^{d-2} \ln K + \ldots], \tag{16}$$

so that $K = \mathrm{O}(\Delta\rho)^\nu$ with $\nu = 1$ for $d = 3$, $\nu = \frac{1}{2}$ for $d = 4$. Similarly, with mean cluster size given by

$$S(\rho) = 1 + \rho\tilde{h}^+(\mathbf{0}) \tag{17}$$

we find $S^{-1} = \mathrm{O}(K^2) = \mathrm{O}(\Delta\rho)^\gamma$ so $\gamma = 2\nu$ and $\gamma = 2$ for $d = 3$, $\gamma = 1$ for $d \geqslant 4$. We note also that for $d \neq 4$ we have pure power-law dependence of S and K on $\Delta\rho$ as $\Delta\rho \to 0$ but for $d = 4$ there is also logarithmic dependence, $\Delta\rho \sim K^2 \ln K$. Corresponding calculations for the RCH model yield the same critical exponents. Instead of (15), however, we have from (9) and (14) the percolation density

$$\rho_{\mathrm{P}} = I - 1 \tag{18}$$

for the RCH. The corresponding percolation probability is here given by $p_{\mathrm{P}} = 1 - \exp(-\rho_{\mathrm{P}})$.

The following points bear comment.

(i) From the above analyses it follows that for both models our approximation has the formal structure of a Pólya walk (i.e., unbiased, with nearest-neighbour step) with

$\rho c^+(\boldsymbol{r})$ at ρ_P corresponding to jump probability and $\delta_{r,0}+\rho h^+(\boldsymbol{r})$ corresponding to a generating function that at ρ_P becomes the expectancy of hitting point $\boldsymbol{r}$, starting from $\boldsymbol{r}=\mathbf{0}$. (See Stell (1983) and Cummings and Stell (1983) for a discussion of random walks from this viewpoint.) This correspondence generates a realisable Pólya walk in the case of the RCH model, where $\rho c_0=0$ and $\rho c_1>0$ at ρ_P. In the SP case, $\rho c_0<0$ and $\rho c_1>0$, so the correspondence does not generate a realisable walk. Nevertheless it gives rise, through (15) and the identity $R=(I-1)/I$, to the identity

$$\rho_P = R \tag{19}$$

where R is the probability of return to the original for such a walk. Moreover we see that our MS approximation corresponds to a random walk structure in a way that generates percolation exponents for $d=3$ with values considerably closer to sharp estimates of the exact exponents, $\gamma\approx 1.74$, $\nu\approx 0.86$ (Gaunt and Sykes 1983) than the mean-field values $\gamma=1$, $\nu=\frac{1}{2}$. An analogous point was made by Stell (1969) in connection with the critical-point exponents of a lattice gas in mean-spherical type approximations but is even more pertinent for percolation, since for $d=3$ the percolation exponents are much closer to their MS values than are the critical-point exponents.

(ii) On a simple cubic lattice $\rho_P=R$ yields $\rho_P(d)=0.341\ldots$ for $d=3$ and $\rho_P(4)=0.193\ldots$. Other estimates and discussions of $\rho_P(d)$ suggest the values $\rho_P(3)\approx 0.312$ to within 1% and $\rho_P(4)\approx 0.197$ to within 3%. Thus our $\rho_P(4)$ appears competitive with the best available results. For larger d, we analyse our approximation using the method suggested by Gaunt and Brak (1984) to test such results. We compare the expansion of R in σ^{-1}, $\sigma=2d-1$, with that of ρ_P (Gaunt *et al* 1976) and find $(\rho_P-R)/\rho_P=(2\sigma)^{-1}+O(\sigma^{-2})$. Together with our analysis for $d=3$ and 4 this supports $\rho_P>R$ for $d\geqslant 4$, $\rho_P<R$ for $d\leqslant 3$, and shows that the inequality $R>\rho_P$ proposed by Ishioka and Koiwa (1978) for all d is without support.

(iii) For $d=1$, our SP result yields

$$\delta_{r,0}+\rho h^+(\mathbf{r})=\rho^r, \tag{20}$$

$$1+\rho\tilde{h}^+(\boldsymbol{k})=(1-\rho^2)/[1-2\rho\cos k+\rho^2], \tag{21}$$

so from (15)

$$S(\rho)=(1+\rho)/(1-\rho). \tag{22}$$

These are exact results. Our approximation is also exact for SP on a Bethe lattice, where (19) and (20) continue to hold with r now equal to path length from origin. For $\rho<\rho_P=(z-1)^{-1}$, $S(\rho)$ from (20) through (15) immediately generalises to the exact result

$$S(\rho)=(1+\rho)/[1-(z-1)\rho]. \tag{23}$$

(We defer further discussion of the Bethe-lattice results to a less space-restricted treatment elsewhere.)

(iv) For the RCH, we have from (18) $p_P(3)=0.403\ldots$ and $p_P(4)=0.213\ldots$ but we do not expect these values to approach the accuracy of our simple cubic SP results, on the basis of a detailed ongoing quantitative study of the continuum analogue of the RCH by Chiew and Stell. On the basis of that study, however, we expect the RCH $p_P(d)$ obtained from the first correction given by (27) below to be highly accurate.

(v) In Stell (1984) the correction to the SU/PY result for $c^+(\boldsymbol{r})$ was given through order ρ^2. For our SP and RCH models one has, from equations (9) and (10) of Stell (1984),

$$c^+(\boldsymbol{r}) = d^+(\boldsymbol{r}) \qquad \text{for } r > 1, \tag{24}$$

where

$$d^+(\boldsymbol{r}) = \rho^2 d_2^{+(2)} + \mathrm{O}(\rho^3) \tag{25}$$

with $d_2^{+(2)}$ given by the right-hand side of (11) of Stell (1984). In the SP model, hole-particle symmetry implies that $d^+(\boldsymbol{r})$ is invariant under the mapping $\rho \to -\rho$, so that $\rho(1-\rho)$ rather than ρ is a natural expansion parameter. Here $\rho\Omega$ can be equally well identified as occupation probability p or volume fraction ϕ of occupied lattice cells with cell volume Ω. Thus the approximant of $d^+(\boldsymbol{r})$ that is suggested by symmetry is

$$d^+(\boldsymbol{r}) = \phi^2(1-\phi)^2 d_2^{+(2)}. \tag{26}$$

In the RCH case, hole-particle symmetry is lost, and ϕ is the natural parameter of smallness (where now $\phi = p = 1 - \mathrm{e}^{-\rho\Omega}$). Hence

$$d^+(\boldsymbol{r}) = \phi^2 d_2^{+(2)} \tag{27}$$

is an appropriate form, with the further simplification that $d_2^{+(2)}$ in the RCH case is given by the right-hand side of (18) of Stell (1984).

(vi) Since the standard bond percolation problem on a regular lattice can be transformed into an equivalent site percolation problem on an associated covering lattice, our method is applicable to bond percolation problems as well. This transformation will yield results in terms of the lattice Green function of the covering lattice. An intriguing question is whether an alternative mapping exists that will yield OZ bond percolation results directly in terms of the Green function of the primary lattice, permitting contact with observations of Sahimi *et al* (1983).

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