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LETTER TO THE EDITOR

Monte Carlo tests of universality in a correlated-site percolation problem

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Abstract. We study a correlated-site percolation model on a square lattice in which a site is occupied if all four bonds surrounding it are occupied; this model is of possible relevance to supercooled H_2O and D_2O. Using Monte Carlo methods, we find the critical concentration of sites $p_c = 0{\cdot}562 \pm 0{\cdot}001$, and the critical exponents $\nu = 1{\cdot}33 \pm 0{\cdot}07$ and $\gamma = 2{\cdot}56 \pm 0{\cdot}27$. These results indicate that this correlated percolation problem is in the same universality class as uncorrelated percolation, while the critical threshold is decreased by about 5% relative to its value for the corresponding random-site percolation problems.

1. Introduction

Recently a correlated-site percolation model has been proposed (Stanley 1979, Stanley and Teixeira 1980) that is possibly of relevance in providing some insight into the behaviour of supercooled H_2O and D_2O (Angell 1980)§. A fraction p_B of bonds are randomly occupied, and then the sites are partitioned into $z+1$ separate species ('colours') according to the number $j = 0, 1, 2, \ldots, z$ of bonds emanating from each site; z is the coordination number. Although the fraction of sites f_j belonging to species j is determined solely by the random variable p_B,

$$f_j = \binom{z}{j} (p_B)^j (1-p_B)^{z-j}, \tag{1}$$

the connectivity properties are very different from those of pure percolation. For example, if the z nearest neighbours of a given site belong to species z, then the site itself must be species z.

This 'polychromatic correlated-site percolation problem' is of theoretical interest in its own right, independent of its possible utility in providing a physical mechanism germane to supercooled water, because it is a simple example of correlated-site percolation. Previous studies of correlated-site percolation have concerned the connectivity of spins which are partitioned into two classes—'up' or 'down'—on the basis of an Ising or lattice-gas interaction (see e.g. Coniglio *et al* (1979), Stoll and Domb (1979) and references therein). The present model is far easier to study because it

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§ Correlated-site percolation refers to the study of the connectivity of objects whose state is not randomly determined, as in random-site percolation.

begins with random bond occupancy. One open question is whether or not critical-point exponents are the same for this correlated-site percolation problem as for random percolation, that is, whether or not the two problems are in the same universality class. This is the question addressed here.

We treat the square lattice ($z = 4$) and consider the somewhat simpler 'bichromatic' problem in which the $z + 1$ different site species are divided into two classes. A site is a member of the first class (and is indicated by a heavy dot) if all z bonds emanating from it are occupied, as shown in figure 1. All other sites belong to the second class; these are not marked. Nearest-neighbour four-bonded sites are said to belong to the same cluster. It is our object to study the nature of the singularities in the various cluster properties as the site density $\rho \equiv f_4 = (p_B)^4$ approaches ρ_c, the percolation threshold. To this end, we employ Monte Carlo computer simulation procedures for the square lattice with L sites on its edge, where L ranges from 20 to 300. Periodic boundary conditions are used, so that the lattice is in reality a torus; we say that a given finite $L \times L$ system 'spans' if there is a cluster which surrounds the hole in the torus. The amount of data generated for each value of ρ ranges from 1000 realisations at $L = 20$ and $L = 40$, to 120 realisations at $L = 300$.

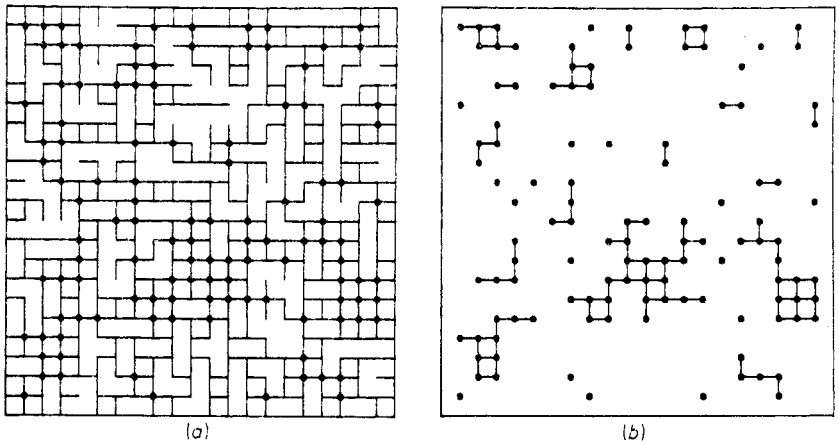

Figure 1. The determination of the site clusters. A site is occupied if and only if all four bonds surrounding it are occupied. Shown is one realisation for $L = 20$ (the smallest of the size sequence studied here), with $p_B = 0{\cdot}75$; hence $\rho = p_B^4 \cong 0{\cdot}32$, well below the percolation threshold. Site clusters in (a) are displayed more clearly in (b) in which all bonds which do not connect nearest-neighbour sites have been removed. Samples of size up to $L = 300$ were used in the present Monte Carlo study.

2. Estimation of ρ_c and the critical exponents ν and γ

We define $\pi(\rho)$ as the percentage of realisations which span at a site concentration ρ. In figure 2(a) we plot $\pi(\rho)$ for sizes $L = 20, 40, 50, 100, 200$, and 300. With increasing cell size, the function $\pi(\rho)$ approaches a step function, where $\pi(\rho) = 0$ for $\rho < \rho_c$ and $\pi(\rho) = 100$ for $\rho > \rho_c$. Defining ρ_{20} and ρ_{80} as the site concentrations at which respectively 20% and 80% of all realisations span, it is quite apparent from figure 2(a) that ρ_c lies between ρ_{20} and ρ_{80} for all cell sizes studied.

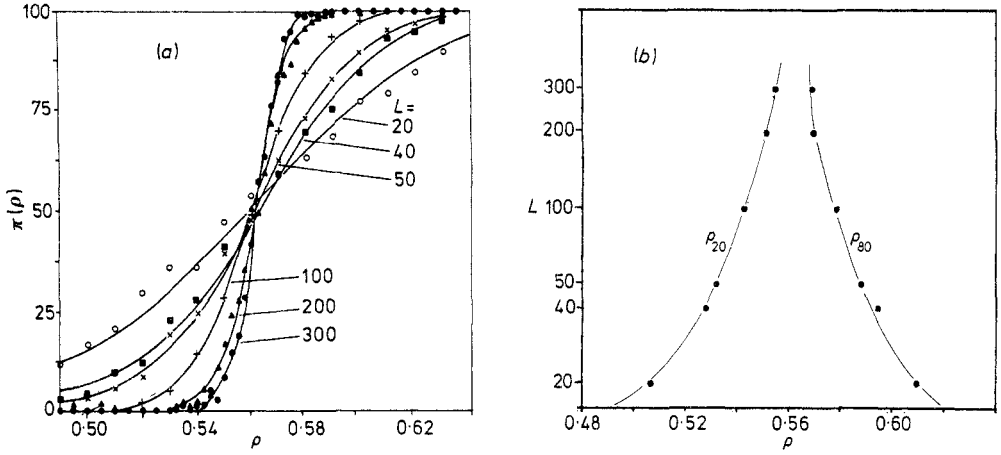

Figure 2. (*a*) A plot of $\pi(\rho)$, the percent span, for $L = 20, 40, 50, 100, 200$ and 300. With increasing cell size, $\pi(\rho)$ approaches a step function, where $\pi(\rho) = 0$ for $\rho < \rho_c$ and $\pi(\rho) = 100$ for $\rho > \rho_c$. (*b*) A plot of lg L against ρ_{20} and ρ_{80}. Because ρ_{20} approaches ρ_c from below and ρ_{80} approaches ρ_c from above, ρ_c lies somewhere in the region between $\rho_{20}(L = 300)$ and $\rho_{80}(L = 300)$; i.e. $0{\cdot}555 < \rho_c < 0{\cdot}565$. ρ is the site density.

In figure 2(*b*) is plotted lg L against ρ_{20} and ρ_{80}†. The values ρ_{20} and ρ_{80} for $L = 300$ define a narrow range for the value of ρ_c, $0{\cdot}555 < \rho_c < 0{\cdot}569$. An eyeball extrapolation of the two curves provides a rough estimate of $\rho_c \cong 0{\cdot}562$.

From finite-size scaling theory (Fisher 1971, Sur *et al* 1976), we expect

$$\rho_{20}(\infty) - \rho_{20}(L) \sim L^{1/\nu} \qquad \rho_{80}(L) - \rho_{80}(\infty) \sim L^{1/\nu'} \tag{2}$$

where $\rho_{20}(\infty) = \rho_{80}(\infty) = \rho_c$, and ν is the connectedness length exponent. In figure 3(*a*), the plot of $\lg(\rho_{20} - \rho_c^{\text{trial}})$ and $\lg(\rho_{80} - \rho_c^{\text{trial}})$ against lg L yields the exponents ν' and ν which refer to the connectedness length singularity above and below ρ_c respectively. Choosing ρ_c through a least-squares fit such that $\nu = \nu'$, we find $\rho_c = 0{\cdot}562 \pm 0{\cdot}001$, and

$$\nu = \nu' = 1{\cdot}33 \pm 0{\cdot}11. \tag{3a}$$

This procedure has the drawback that ν depends on ρ_c^{trial}, which must be chosen in some fashion. An alternative procedure is to plot $\lg(\rho_{80} - \rho_{20})$ against lg L, as in figure 3(*b*). From the slope of the straight line shown, we obtain the estimate

$$\nu = 1{\cdot}33 \pm 0{\cdot}07. \tag{3b}$$

Both estimates, (3*a*) and (3*b*), compare favourably with values reported for random site percolation: $\nu = 1{\cdot}32^{+0{\cdot}02}_{-0{\cdot}07}$ (Cox and Essam 1976), $\nu = \ln(3^{1/2})/\ln(3/2) \cong 1{\cdot}354$ (Klein *et al* 1978), $\nu = \frac{4}{3}$ (den Nijs 1979), and $\nu = 1{\cdot}354 \pm 0{\cdot}015$ (Reynolds *et al* 1978, 1980).

The critical behaviour of the mean cluster size, $S(\rho)$, is described by the exponents γ and γ',

$$S(\rho) \sim \begin{cases} C_+(\rho - \rho_c)^{-\gamma} & \rho < \rho_c \\ C_-(\rho_c - \rho)^{-\gamma'} & \rho > \rho_c \end{cases} \tag{4}$$

† For a parallel treament of random-site percolation, see Roussenq *et al* (1976).

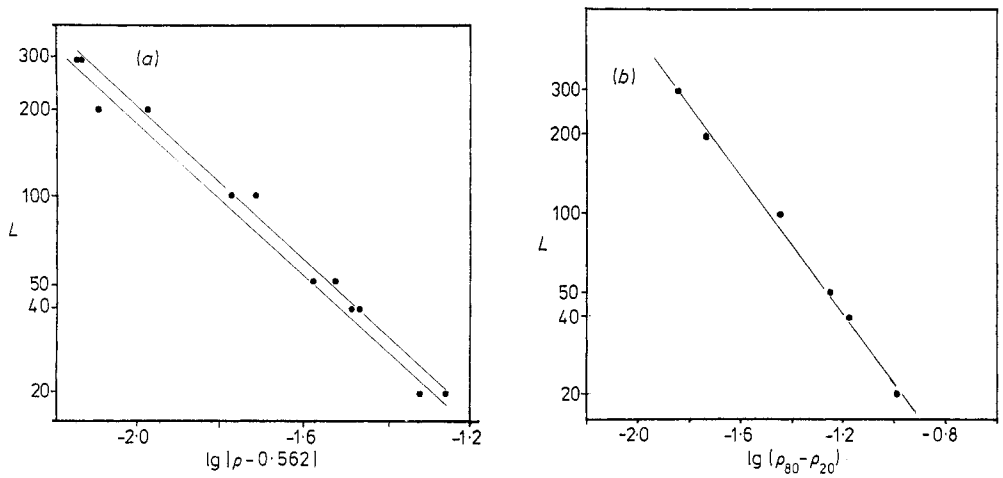

Figure 3. (*a*) A plot of lg L against lg $|\rho_c - \rho_{20}|$ and lg $|\rho_{80} - \rho_c|$. Since $(\rho - \rho_{20}) \sim L^{1/\nu}$ and $(\rho_{80} - \rho_c) \sim L^{1/\nu'}$, the slopes of the two curves are ν and ν' respectively. Choosing ρ_c according to the self-consistent criterion that $\nu = \nu'$, we find that $\rho_c = 0{\cdot}562$ and $\nu = \nu' = 1{\cdot}33$. (*b*) A plot of lg L against lg $(\rho_{80} - \rho_{20})$. The straight line has slope $= -\nu = -1{\cdot}33$.

A least-squares fit of lg $S(\rho)$ against lg $|\rho - \rho_c|$, where $S(\rho)$ includes the largest cluster only for $\rho < \rho_c$, yields slope $-\gamma$ for $\rho < \rho_c$ and slope $-\gamma'$ for $\rho > \rho_c$. Choosing ρ_c^{trial} such that $\gamma = \gamma'$, we find $\rho_c = 0{\cdot}564 \pm 0{\cdot}003$ and

$$\gamma = \gamma' = 2{\cdot}56 \pm 0{\cdot}27 \tag{5}$$

for our $L = 300$ data (figure 4(*a*)). The data for smaller sizes are consistent with (5), but display rounding for ρ close to ρ_c. The estimate (5) compares favourably with values reported for random site percolation: $\gamma = 2{\cdot}43 \pm 0{\cdot}03$ (Sykes *et al* 1976a) and $\gamma = 2{\cdot}432 \pm 0{\cdot}035$ (Reynolds *et al* 1978, 1980).

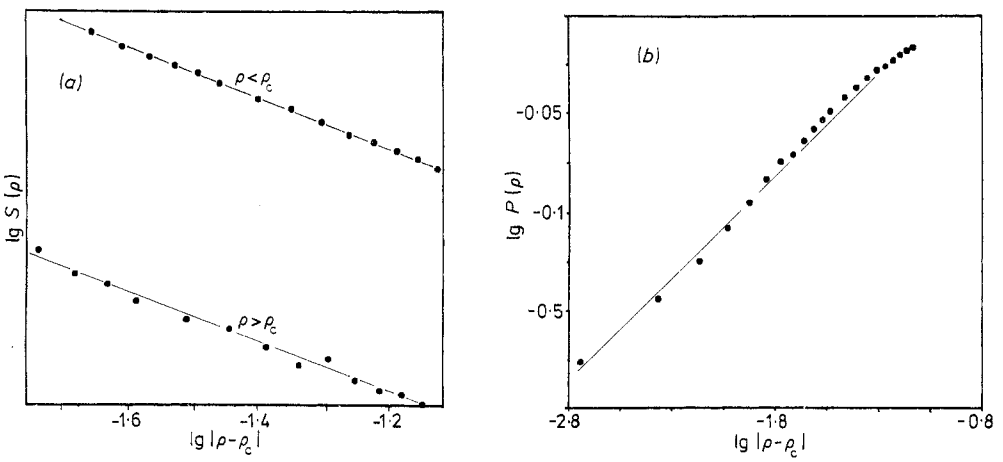

Figure 4. (*a*) A plot of lg $S(\rho)$ (arbitrary units) against lg $|\rho - \rho_c|$ for $L = 300$, where $S(\rho)$ includes the largest cluster only below ρ_c. Choosing a trial ρ_c such that $\gamma = \gamma'$, we find $\rho_c = 0{\cdot}564$ and $\gamma = \gamma' = 2{\cdot}56$. (*b*) A plot of lg $P(\rho)$ against lg $|\rho - \rho_c|$, where $P(\rho)$ is the fraction of sites in the largest cluster. By varying ρ_c to get the best linear fit, we find $\beta = 0{\cdot}104$ and $\rho_c = 0{\cdot}561$.

The lg–lg plots in figure 4(a) also give the amplitude ratio C_+/C_-. We find

$$C_+/C_- = 280{\cdot}4 \pm 65. \tag{6}$$

This value may be compared with the literature estimates $C_+/C_- = O(1)$ (Sykes *et al* 1976a, b), $C_+/C_- = 196 \pm 40$ (Hoshen *et al* 1979), and $C_+/C_- = 219 \pm 25$ (Nakanishi and Stanley 1980).

3. Discussion

We conclude with some discussion of the value of ρ_c for the correlated-site problem. We recall from §2 that eyeball extrapolation of figure 2(b) gives $\rho_c = 0{\cdot}562$, and figure 3(a) gives $\rho_c = 0{\cdot}562$ while figure 4(a) gives $\rho_c = 0{\cdot}564$. However, the data of figure 4(a) are for only one cell size ($L = 300$); hence we are inclined to weight this estimate rather less than the others. Based on the analysis presented above (and a variety of other considerations), we conclude that the best estimate of ρ_c is

$$\rho_c = 0{\cdot}562 \pm 0{\cdot}001. \tag{7}$$

Thus far we have discussed only two critical exponents, ν and γ. The values we obtained are within the error bars of most literature estimates for random percolation; hence we conclude that there is no evidence to suggest that the correlated-site problem is in a different universality class than random-site percolation.

Other percolation functions were also studied, but the accuracy obtained with the Monte Carlo information available was not sufficient to provide reliable information. For example, $P(\rho)$, the fraction of occupied sites in the largest cluster, varies as $P(\rho) \sim |\rho - \rho_c|^{\beta}$. Using $P(\rho)$ data for $L = 300$, we vary ρ_c^{trial} to get the best linear fit; we find $\rho_c = 0{\cdot}561 \pm 0{\cdot}003$ and $\beta = 0{\cdot}104 \pm 0{\cdot}020$ (figure 4(b)). The series estimate is $\beta = 0{\cdot}138 \pm 0{\cdot}007$ (Sykes *et al* 1976b) and the large-cell PSRG estimate is $\beta = 0{\cdot}138^{+0{\cdot}005}_{-0{\cdot}006}$ (Reynolds *et al* 1978, 1980).

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Note added in proof. Very recently, Brodsky (1980a,b) has found that the present model may be suitably adapted to explain a wide range of anomalous behaviour occurring in hydrogenated amorphous Si (a – Si : H), an amorphous semiconductor characterised by 'patches' of pure Si (a – Si), bounded by hydride regions (a – SiH_x).

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