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Correlated two-component percolation

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Abstract. A correlated two-component percolation model is constructed to treat random bonds between next-nearest neighbours. Monte Carlo simulations on a 2D square lattice are performed. By employing real-space renormalization techniques, it is proved that the criticality is controlled by a single fixed point and the percolation exponents are unaffected by correlations. The discovered power law dependence with exponent $1/\nu$ of the percolation threshold p_c on the concentration of the second phase is discussed.

Percolation theory has received much attention in recent years, partly because it provides a simple geometrical interpretation of phase transitions and also because of its direct relevance to various physical phenomena. (See, e.g., Essam 1980, Stauffer 1985 for recent reviews.) The two classical versions are the site and the bond percolation. More general models, such as site-bond (Shapiro 1979), directed bond (Blease 1977), and polychromatic (Deutscher 1983, Zallen 1977) percolation, have recently been introduced.

In the present paper another generalization is considered, the contributions of the correlated next-nearest neighbour bonds to the cluster formation on a 2D square lattice. In the method every site can be independently occupied by a particle of type A (referred to hereafter as 'black particle') or of type B ('grey particle'), or be empty, with probability p, g and $1-p-g$, respectively. Similarly to the ordinary site percolation problem, all black sites in nearest neighbour positions are assumed to be connected and form clusters (see figure 1). The grey particles affect the percolation path by adding diagonal links between its four adjacent lattice sites. For example the box shown in figure 1(b) percolates, while the chain 1(c) does not. Thus the lattice pattern consists of randomly distributed regions of site and bond defined clusters, which interact via common interfaces. This model is reminiscent of the two-component bond problem studied by Bunde *et al* (1985), but the black cluster ramification is not fixed. We believe that the correlated two-component percolation as introduced reflects more precisely the physics of layer formation in the presence of active centres (Evans and Sanders 1989) as well as the role of dispersed insulating phase in composite superionics (Poulsen 1985).

In particular we aim to determine the conditions for criticality.

Monte Carlo (MC) simulations were carried out in order to study the cluster formation dependence on concentration of the active centres (grey particles). 2D square lattices of size $L \times L$, with $L = 800$, 1200, 1600 and 2000 were used. Each MC step with a given set of probabilities (p, g) started with assigning the lattice. A site was considered

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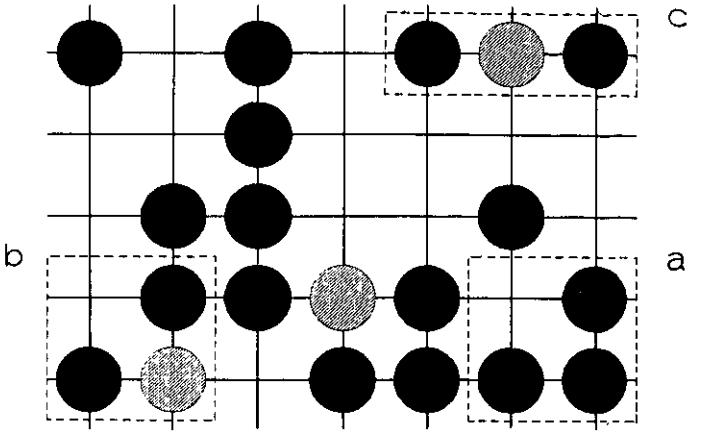

Figure 1. Cluster formation rules. Box (a) percolates via nearest neighbour links (ordinary site percolation); box (b) percolates via diagonal link provided by the grey site; no coupling between black sites exists in box (c). The pattern shown percolates in both horizontal and vertical directions.

to be occupied by a black particle if the random number r is less than p, where $r \in [0, 1)$, by a grey particle if $p \leq r < p+g$, or unoccupied if $r \geq p+g$. Several runs at different configurations were performed to improve the statistics. Preliminary calculations by the small-cell position space renormalization group (PSRG) were made to localize the percolation threshold $p_c(g)$. Varying p in the vicinity of this zero-order approximation for p_c (10 values below and 10 values above with average step of 0.003), cluster enumerations were carried out by employing the technique of Hoshen and Kopelman (1976), which has been proved to be extremely efficient for large lattices.

Following Hoshen *et al* (1987) the percolation probability P (the fraction of black sites belonging to the largest cluster) and the susceptibility χ (the mean cluster size) were approximated by:

$$P = \frac{1}{G} s_{\max} \qquad \chi = \frac{1}{G}\left(\sum_s s^2 n_s - s_{\max}^2\right) \tag{1}$$

where n_s is the number of clusters of size s, $s_{\max}$ is the size of the largest cluster and $G = \Sigma_s s n_s$ is the total number of black sites. The percolation threshold p_c was identified with the position of the peak in the $\chi = \chi(p)$ curve.

The concentration g of the grey particles was varied from $g = 0$ to $g = 0.593$ (for $g \geq 0.593$ an infinite grey cluster exists and no black percolation is possible). Results for p_c are shown in table 1. Each value was estimated by averaging over $16 \div 64$ MC runs. For the lower limit $g = 0$, the value of $p_c = 0.593$ confirms the result for the square lattice. For the upper limit $g \to 0.593$, p_c asymptotically approaches 0.407 which is the

Table 1. Monte Carlo results for the percolation threshold $p_c(g)$, where g is the grey sites concentration.

g	0.01	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.50	0.55	0.58
p_c	0.582	0.555	0.525	0.495	0.475	0.470	0.448	0.440	0.420	0.410	0.408	0.407

percolation threshold value for a system with both nearest and next-nearest neighbour interactions (Stauffer 1985).

The PSRG method was employed in determining the critical parameters of the system in a version that extends previous studies by Reynolds *et al* (1977, 1978) and Shapiro (1979). The most simple approach is to consider a RG procedure that keeps the renormalized nodes uncorrelated, i.e. the two different probabilities for site occupation p, g to be worked out separately. The lattice was partitioned into cells consisting of four sites (rescaling factor $b=2$), each cell scaled to a single site. The renormalized black-occupation probability p' was obtained by summing up the probabilities of all horizontally percolated cells. All configurations which provide diagonal links for the adjacent cells but do not percolate themselves were assumed to contribute to g' (cf figure 2). Then it was straightforward to derive the recursion relations:

$$p' = -p^4 - 4p^3 g + 2p^2(1 + 2g - g^2) \tag{2a}$$

$$g' = -2g^3 + g^2(3 - 2p^2) \tag{2b}$$

$$1 \geqslant p + g \tag{2c}$$

where the last equation defines the physical region of (p, g)-plane. The equations (2) solved together lead to the flow diagram shown in figure 3. There are six fixed points: three trivial fixed points $(p, g) = (0, 0)$, $(1, 0)$ and $(0, 1)$, two fixed points $(0.618, 0)$ and $(0, 0.5)$, that correspond to the pure one-component site and bond percolations respectively, and a new fixed point at $(0.38, 0.62)$. There are two critical lines starting from this point and reaching both fixed points $(0.618, 0)$ and $(0, 0.5)$. The exponents ν evaluated with the help of the linearized equations (2) were found to be 1.63 at both fixed points $(0.618, 0)$ and $(0.38, 0.62)$. This is consistent with the estimation obtained by Reynolds *et al* (1977) for four-site approximation. Therefore, the correlation does not affect the critical exponents which are the same as for the site and the bond problems in accordance with the concept of universality (Shapiro 1979). This conclusion

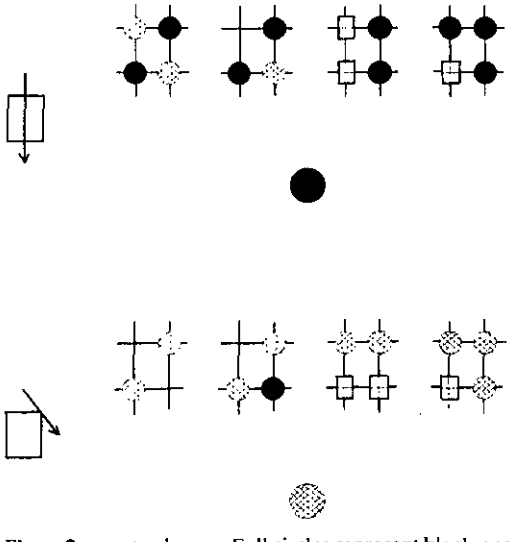

Figure 2. PSRG schemes. Full circles represent black-occupied sites, shaded circles represent grey sites, and boxes correspond to threefold degenerate sites, i.e. black, grey, or empty.

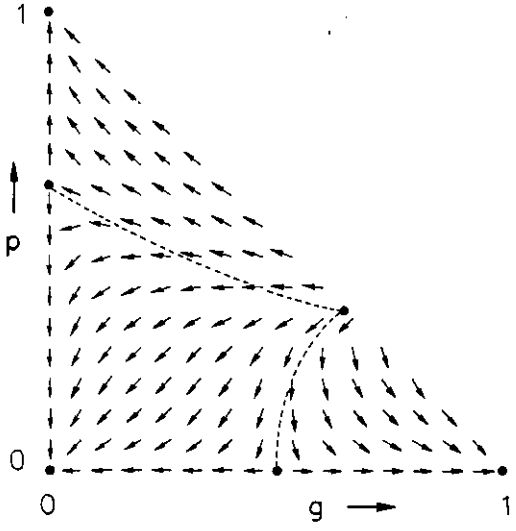

Figure 3. The flow diagram. Full circles mark the fixed points. The critical lines separate the percolating and non-percolating regions in the parameter plane.

was confirmed by the finite-size scaling plots

$$P_L = L^{-\beta/\nu} f[(p-p_c)L^{1/\nu}] \tag{3a}$$

$$\chi_L = L^{\gamma/\nu} h[(p-p_c)L^{1/\nu}] \tag{3b}$$

where typical values of $\beta = \frac{5}{36} = 0.138$, $\gamma = \frac{43}{18} = 2.4$ and $\nu = \frac{4}{3}$ were used. Here L is the lattice size, f and h are suitable scaling functions. The MC patterns for P_L and χ_L taken at $g = 0.1$ are shown in figures 4 and 5, respectively. The data collapse is relatively good.

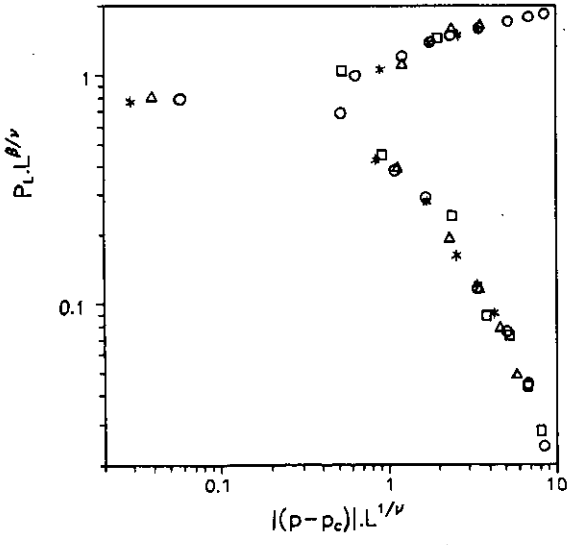

Figure 4. The finite size scaling function $P_L L^{\beta/\nu}$ shown as a function of $|p-p_c|L^{1/\nu}$. L is the linear size of the lattice from 800 (*), 1200 (△), 1600 (◇) and 2000 (○). P_L is the percolation probability (the fraction of black sites, belonging to the largest cluster). The concentration of grey particles g is taken 0.1.

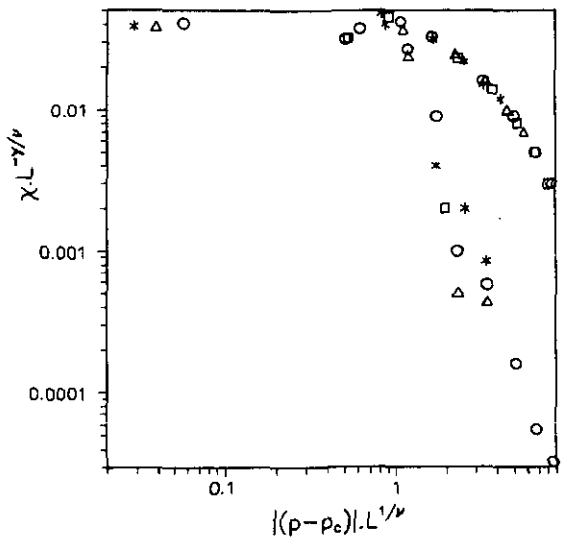

Figure 5. The finite size scaling function $\chi_L L^{-\gamma/\nu}$ shown as a function of $|p-p_c|L^{1/\nu}$. L is the linear size of the lattice from 800 (*), 1200 (△), 1600 (◇) and 2000 (○). χ_L is the *susceptibility (the mean cluster size)*. The concentration of grey particles g is taken 0.1.

On the other hand the study of percolation threshold p_c revealed a surprising power law dependence on concentration of the grey particles. The data obtained from MC experiments are presented in table 1 and the best fit (see figure 6) gives

$$p_c(g=0)-p_c(g) \propto g^{1/\nu}. \tag{4}$$

This relation could find an explanation in terms of scaling properties of the system in the vicinity of the percolation threshold. An important feature for the model

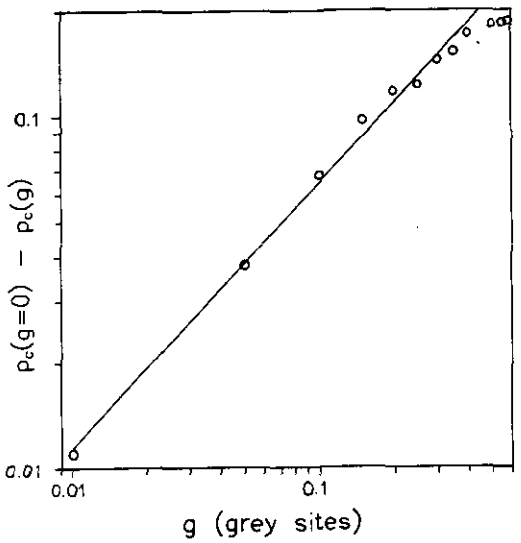

Figure 6. The shift of the percolation threshold $p_c(g)$ as a function of grey sites concentration.

considered is the presence of two length scales: the correlation length ξ_0 when the diagonal bonds are removed, and the correlation length ξ, when all links are taken into account. Let us consider the probability $P(r)$ to have a cluster of size r, which is composed of smaller pure black clusters of size r_i ($\Sigma r_i = r$) joined by grey particles:

$$P(r) \sim \exp(-r/\xi) = \sum_{m \in \Gamma} g^m \prod_i P_0(r_i)$$

$$\sim \exp(-r/\xi_0) \sum_{m \in \Gamma} g^m \approx \frac{\exp(-r/\xi_0)}{1-g} \tag{5}$$

where the summation is over all possible configurations Γ, and $P_0(r_i)$ is the probability of a pure black subcluster of size r_i. The approximation made in the equation (5) is valid for small concentration of grey-occupied sites $g \ll 1$. Taking the logarithm from both sides of (5) one obtains

$$\frac{-r}{\xi} = \frac{-r}{\xi_0} - \ln(1-g) \qquad \text{or} \qquad \xi = \frac{\xi_0}{1 - g\xi_0/a} \tag{6}$$

where for the normalization constant is accepted the lattice spacing a. Since at $p \to p_c(g)$ the correlation length ξ diverges as $|p - p_c(g)|^{-\nu}$ and ξ_0 is finite, the dependence (4) follows after simple calculations.

In conclusion we have introduced a generalized two-component percolation problem accounting for random bonds between next-nearest neighbours. We have developed a RG scheme which enables us to obtain the phase diagram and to demonstrate that the problem belongs to the same universality class as the ordinary site and bond percolation. In addition we have discovered a power law dependence with exponent $1/\nu$ of $p_c(g=0) - p_c(g)$ on the concentration g of the second phase.

The possibility to control the intrinsic length of the system by changing the impurity density is very attractive for practical applications. It could be helpful in understanding the physical phenomena like adsorption, superconductivity in granular materials, ionic conductivity in dispersed solid electrolytes, etc.

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