Critical exponents for site-bond-correlated percolation

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We examine a limiting case of the percolation model with site-bond correlation used in the description of the magnetic behavior of $KNi_pMg_{1-p}F_3$. In this limit, a vacant site destroys the bond between a nearest-neighbor pair along the line joining the three sites. Monte Carlo simulations for both the square and triangular lattices are used to calculate the concentration thresholds and the critical exponent τ describing the scaling of cluster numbers; the latter is related to the order-parameter exponent β. We find that the critical exponents are the same as those for uncorrelated percolation.

In the usual percolation problem,[1] a given site (or bond) is randomly occupied with a certain probability p, *independently* of the configuration of its neighboring sites (and/or bonds). One is then interested in determining critical concentrations and exponents, as well as to establish the scaling properties of macroscopic quantities of interest such as the number of clusters of size s, n_s, the order parameter (the fraction of sites belonging to the infinite cluster), $P(p)$, the average cluster size, $S(p)$, and so on.[1]

The study of some disordered systems in recent years, however, has suggested that uncorrelated disorder was unable to account for all expected properties, so that different models of *correlated* disorder have been proposed. These models can be broadly classified according to the correlation being long or short ranged. Examples in the first category are thermally induced models[2,3] and the bootstrap percolation model,[4] whereas in the second group are high-density percolation[5] and site-bond-correlated models;[6-8] see also Ref. 9 for related work.

The results available so far suggest that the effects of long-ranged correlations are quite drastic: one finds new exponents[3] and, in some cases, first-order transitions;[4] they can also turn the temperature for correlated dilution problems into an irrelevant (in the renormalization-group sense) field near zero temperature.[4(d)] In contrast, short-ranged correlations are unlikely to give rise to a connectivity exponent ν distinct from the uncorrelated case. Physically, the connectivity properties of the percolating cluster are determined by its backbone which, in principle, is not too sensitive to correlations, provided they are short ranged. On the other hand, the mass of the percolating cluster can be affected by correlations, since the dangling bonds contribute to the behavior of $P(p)$ and therefore to that of the critical exponent β. Thus, there is no reason *a priori* to discard the possibility of having $\nu_{\text{corr}}=\nu_{\text{uncorr}}$ while $\beta_{\text{corr}}\neq\beta_{\text{uncorr}}$ for a particular correlation model.

Here, we examine the critical exponents for the so-called site-bond-correlated percolation problem[6-8] in both the square and triangular lattices through Monte Carlo simulations. This model was proposed by de Aguiar *et al.*[6] to explain some unusual experimental results on $KNi_pMg_{1-p}F_3$. First, the decrease in the critical temperature T_c, as the concentration p of magnetic ions is lowered from one is faster for this compound than for the isostructural $KMn_pMg_{1-p}F_3$, which is well described by a standard (noncorrelated) diluted Heisenberg model. Second, the phase boundary between antiferro- and paramagnetic phases in the temperature-concentration plane for $KNi_pMg_{1-p}F_3$ displays an upward curvature, which is absent in its counterpart for $KMn_pMg_{1-p}F_3$. As the magnetic behavior of pure $KNiF_3$ is well described by the Heisenberg model, the observed features have been interpreted as signaling correlated dilution effects.[6] Indeed, the authors of Ref. 6 recall that, while in Mn^{2+} the electronic configuration is such that these ions can form both σ and π bonds with the fluorine ligands, the corresponding configuration in Ni^{2+} ions is such that they can only form σ bonds. Due to the directionality of σ bonds, if a nonmagnetic atom replaces an Ni^{2+} ion, this will strongly affect the interaction of two nearest-neighbor Ni^{2+} along the line joining the three atoms. Those authors then proposed a model with the following expression for the exchange constant between two nearest-neighbor sites:

$$J_{i,i+\delta}=J_{\epsilon_i\epsilon_{i+\delta}}[(1-\alpha)\epsilon_{i-\delta}\epsilon_{i+2\delta}+\alpha]\ , \tag{1}$$

where δ denotes an elementary lattice vector, ϵ_i is a site (random) occupation variable which equals 1 or 0 with probability p or $(1-p)$, respectively. As we are interested in the geometrical properties of the correlated problem, we set $\alpha=0$ so that the bond between i and $i+\delta$ only exists if both sites $i-\delta$ and $i+2\delta$ are occupied. If $0<\alpha<1$, the bond between i and $i+\delta$ is merely weakened by the absence of a magnetic ion at $i-\delta$ or $i+2\delta$, and the disorder is effectively uncorrelated as far as geometrical properties are concerned. Previous studies of this percolation model[6-8] have concentrated on the square lattice and estimates were obtained for p_c and ν. Although the latter was found to be approximately the same as that of uncorrelated percolation, we feel that further investigation is in order, in particular to obtain β. In this way, more complete statements can be made with respect to universality classes. In what follows, we briefly review both the scaling theory of cluster numbers, as well as the Monte Carlo algorithm for percolation problems.

We then present our results and conclusions.

Let us first define n_s as the number of clusters (per lattice site) with s sites. It is by now well established for uncorrelated percolation that, in the asymptotic region $s \to \infty$ and $p \simeq p_c$, one has (see, e.g., Ref. 1)

$$n_s(p) = s^{-\tau} f((p - p_c)s^{\sigma}) , \tag{2}$$

where τ and σ are critical exponents, and $f(z)$ is a scaling function. A log-log plot of n_s at p_c can be used to extract the exponent τ. Given the cluster size distribution, n_s, one can calculate the fraction of sites belonging to the infinite cluster,

$$P(p) = \sum\nolimits'_s [n_s(p_c) - n_s(p)]s \xrightarrow[p \to p_c]{} |p - p_c|^{\beta}$$

(the prime denotes exclusion of the infinite cluster), which plays the role of the order parameter; other quantities may be calculated as different moments of the distribution.[1] With the use of hyperscaling, one can easily get[1]

$$\beta = d\nu \frac{\tau - 2}{\tau - 1} . \tag{3}$$

Since a calculation of β that is both direct and accurate is very hard even for the uncorrelated case (see e.g., Ref. 1), one can use Eq. (3) instead. Our strategy for the correlated case consists in taking ν to be the same as in uncorrelated percolation, as discussed in Ref. [7], and determining τ independently by Monte Carlo simulations.

The simulations can be outlined as follows. A configuration is generated by initially occupying each site of a lattice (of linear size L and with periodic boundary conditions) at random with probability p. For the correlated case one tests if every pair of occupied neighboring sites is such that their nearest neighbors along the line joining them are also occupied [see Eq. (1)]. If this condition is not satisfied the pair is not connected and they only belong to the same cluster if there is another path linking them. A few technical remarks are worth making at this point. First, we use the Hoshen-Kopelman algorithm[10] to verify if the configuration percolates or not; this is achieved by assigning a label to each site to indicate which cluster it belongs to. Second, with this algorithm there is no need to store the configuration of the whole lattice, but only three lines ($3 \times L$); this should be compared with the case of uncorrelated percolation, in which only one line is needed.[1(b)] By using the fact that the same sequence of random numbers can be reproduced for a given seed, one can determine $p_c(L,i)$, where i labels the run (seed), as the concentration at which a spanning cluster first appears. We repeat this procedure for M runs to obtain the average $p_c(L)$ and the corresponding standard deviation. One should note that this procedure is distinct from the one used in Ref. 11, where the critical concentration is signaled by the decrease in the partial sum of cluster numbers.

The calculation of $n_s(p)$ is carried out by grouping the possible cluster sizes into bins corresponding say, to sizes between 2^k and $2^{k+1}-1$, where $k = 1,2,3,\ldots$. The total number of clusters with sizes in that interval, divided by the size of the interval, is then $n_{\bar{s}} L^2$, where $\bar{s}$ is the geometric mean for that interval.

In order to test the method outlined above, we first investigate the uncorrelated problem on a square lattice, for which very accurate results are available.[1,11] Our estimates for $p_c(L)$ were obtained from $M \sim 100$ runs for $600 \le L \le 1600$, and from $M \sim 10$ for $L = 5000$. The computations were carried out in a 386 microcomputer; one needs typically 10 steps of iteration to find $p_c(L,i)$ to four significant figures, which takes about 4 minutes for $L = 1000$ and 25 hours for $L = 10\,000$.

From finite-size-scaling theory,[12] the shift in critical concentration is given by

$$p_c(L) = p_c(\infty) + AL^{-1/\nu} , \tag{4}$$

where A is a nonuniversal amplitude. The circles in Fig. 1 represent $p_c(L)$ as a function of $L^{-1/\nu}$, with $\nu = \frac{4}{3}$, the exact value;[13] extrapolating to $L = \infty$ one gets $p_c = 0.5930 \pm 0.0002$, which should be compared with $p_c = 0.5927 \pm 0.0001$, as obtained by Rapaport[11] from Monte Carlo simulations on a lattice with $L = 80\,000$. In Fig. 2, we show the cluster numbers n_s as a function of s, for a single run on a lattice of linear size $L = 10\,000$, at $p = 0.593\,05$, which is very close to the extrapolated value of p_c; the slope provides the estimate $\tau = 2.06 \pm 0.02$, which should also be compared with the exact value[13] $\tau = 187/91 \simeq 2.0549$. These results indicate that this procedure yields reliable estimates both for $p_c(\infty)$ and for τ, even though we are using somewhat small lattices. Also, the present estimate for $p(\infty)$ only relies on ν being known, while the one in Ref. 11 assumes a previous knowledge of τ. As argued above, the value of τ is still an open question for short-ranged correlation and one should avoid its use in estimating other quantities.

For the correlated problem the runs are about 1.6 and 2.5 times longer (for the square and triangular lattices, re-

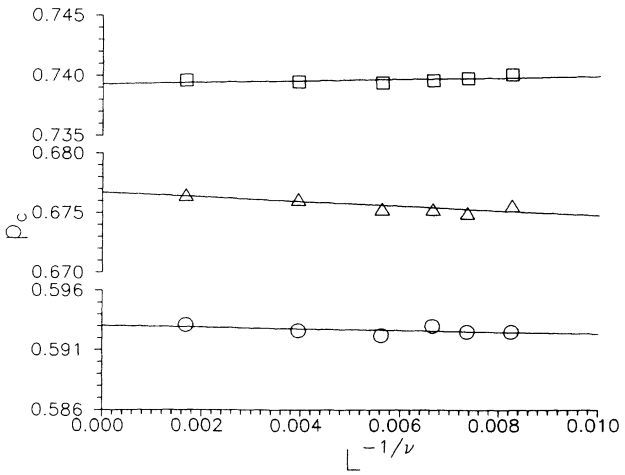

FIG. 1. Average critical concentration as a function of $L^{-1/\nu}$ (L is the linear size of the lattice), for the uncorrelated case on a square lattice (circles), and for the correlated case on the triangular (triangles) and square (square) lattices. The lattice sizes used are $L = 600,700,800,1000,1600,5000$; the error bars are smaller than the data points.

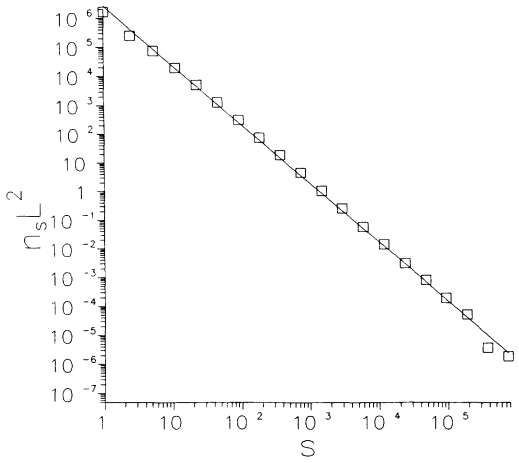

FIG. 2. Cluster numbers [Eq. (2)] at p_c for uncorrelated percolation on a square lattice with $L = 10\,000$.

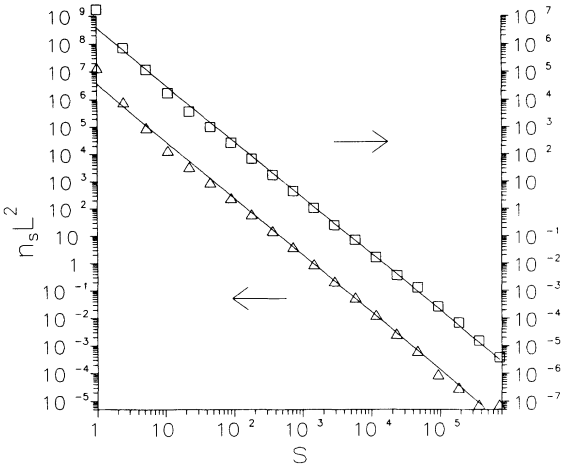

FIG. 3. Cluster numbers [Eq. (2)] at p_c for site-bond-correlated percolation on the square (squares, right axis) and triangular (triangles, left axis) lattices with $L = 10\,000$.

spectively) due to the environmental constraint; the typical number of runs for lattice sizes are the same as for the uncorrelated case. Our results for $p_c(L)$ are also displayed in Fig. 1 (squares and triangles denote the respective lattices) and the extrapolated values are

$$p_c(\text{square}) = 0.7395 \pm 0.0003 ,$$
$$p_c(\text{triangular}) = 0.6768 \pm 0.0002 . \quad (5)$$

For the square lattice, the above value should be compared with $p_c = 0.741 \pm 0.002$, obtained by large-cell position space renormalization group,[7] whereas, to our knowledge, this is the first estimate for the threshold in site-bond-correlated percolation on a triangular lattice. (See Fig. 3).

Our estimates for the cluster number exponent τ, were obtained from lattices with $L = 10\,000$; the runs were carried out at $p = 0.739\,61$ and $p = 0.677\,73$ for the square and triangular lattices, respectively. We get

$$\tau(\text{square}) = 2.03 \pm 0.03 ,$$
$$\tau(\text{triangular}) = 2.07 \pm 0.04 , \quad (6)$$

indicating they are the same, within error bars, as τ for the uncorrelated problem. This suggests that no new universality class is introduced by this correlation.

To summarize, we have calculated percolation thresholds and the exponent describing the scaling of cluster numbers; this exponent is related to β. The procedure used to estimate p_c in all cases turned out to be very reliable, and is intermediate between those used for many runs on small lattices and those for single runs on very large lattices. We can conclude by stating that the range of correlations within this model is too short to give rise to new critical exponents or to modify the scaling form of cluster numbers. The possibility of subdominant (i.e., corrections to scaling[11]) exponents being affected by short-ranged correlations was not examined here due to our limited computer capabilities.

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