Percolation in simple patchwise lattices

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(Received 28 July 1997; revised manuscript received 8 October 1998)

We study the site percolation problem on square lattices with two kinds of sites, which are assembled in such a way that the resulting structures have patchwise topographies. Lattices formed by collections of either randomly or orderly localized patches of different sizes are generated. The composition of this system is specified by two independient variables, p and q, which are the occupation probabilities of each type of patch. Interesting phase diagrams in (p,q) composition space for the percolative transition are obtained and explained. [S1063-651X(99)07602-3]

PACS number(s): 64.60.Ak, 64.60.Cn, 64.70.Pf

Percolation theory has been known for several years and has been extensively reviewed [1–10]. It deals with the effect of random dilution of elementary geometrical object (spheres, sticks, sites, bonds, etc.) located in lattices or in the continuum. Upon dilution of the elements, a sharp transition is found to occur in the connectivity of the system. The percolation threshold is defined as the minimum concentration or density at which an infinite cluster of occupied elements spans the system. The percolation model has many generalizations, which represent diverse physical situations, and has been applied to numerous problems in a large variety of fields. They include correlated percolation, extended-range percolation, directed percolation, polychromatic percolation, etc.

The aim of the present paper is to investigate the site percolation problem in a special lattice with restricted geometry, i.e., the patchwise lattice. These lattices, largely used to model adsorptive heterogeneous surfaces, are composed of two different types of sites, which in turn are grouped into homogeneous patches or finite domains. Our main motivation to study the percolation properties of these structures is based on the fact that previous results of adsorption, diffusion, and reaction on both random [11–13] and ordered patchwise lattices [14–16] have been very interesting from both theoretical and practical points of view.

Let us consider a square lattice of $L\times L$ sites, as a board divided in black (B) and white (W) square patches with each one having l^2 sites. We assume that the number of B squares is the same as the number of W squares. B and W patches can be put in order onto a square lattice, in such a way that any $B(W)$ patch has four nearest-neighbor $W(B)$ patches, so the resulting structure will be a perfect chessboard lattice or regular patchwise lattice. But if the squares in a chessboard are randomly occupied by B or W patches, we have a random patchwise lattice. These lattices can be easily simulated on the computer. We suppose that the patches are touched together, sharing common borders, and any overlap between them is entirely forbidden.

This simple model could represent a ternary material, composed by two conducting species, with conductivities σ_B and σ_W, and an isolating one. Imagine that each site of B (or W) patch is either occupied by a piece of conducting material, with conductivity $\sigma_B(\sigma_W)$ and with probability $p(q)$, or by a piece of isolating material, with probability $1-p(1-q)$. Then, electrical current can flow from one conducting site to another, if both sites are nearest neighbors and no matter which conductivities the sites have. If the occupations p and q are independent, it is possible to analyze the effect that concentrations, and also the size of the patches and their localization (ordered or random) have on the percolation and conduction of the sample. Obviously, the conductance of the sample G depends on concentrations and also on conductivities, i.e., $G=G(p,q,\sigma_B,\sigma_W)$.

Let p and q be the occupation probabilities for a site belonging to the black or white square, respectively. Just as in classical site percolation two adjacent or nearest-neighbor filled sites are considered to be connected to each other, no matter which color the sites have. With both B and W sites occupied at random, the composition of the system is specified by two independent variables p and q. If the network is very large and p and q are sufficiently small, the size of any cluster is likely to be small. But if p and q are close to unity the network should be entirely connected and an infinite cluster of occupied sites spans the network. For a percolation path to occur, both p and q must be large. How large each one must be depends on the other, then p and q are interdependent. The infinite cluster spanning the network will appear only for some well-defined pairs of threshold concentrations $(p_c;q_c)$, then a family of percolation thresholds will arise. The smooth curve defined by the family of pairs $(p_c;q_c)$ represents the phase boundary separating the percolative regime from the nonpercolative one.

Since the lattices prepared on the computer are finites, there will be a certain probability of finding an infinite spanning cluster at any pair (p,q) of occupations. Let p_{av} and q_{av} be the average percolation thresholds for a finite lattice of size L and patches containing l^2 sites. These average thresholds should approach to the real thresholds p_c and q_c in the infinite lattice, i.e, $p_{av}\to p_c$ and $q_{av}\to q_c$ when $L\to\infty$.

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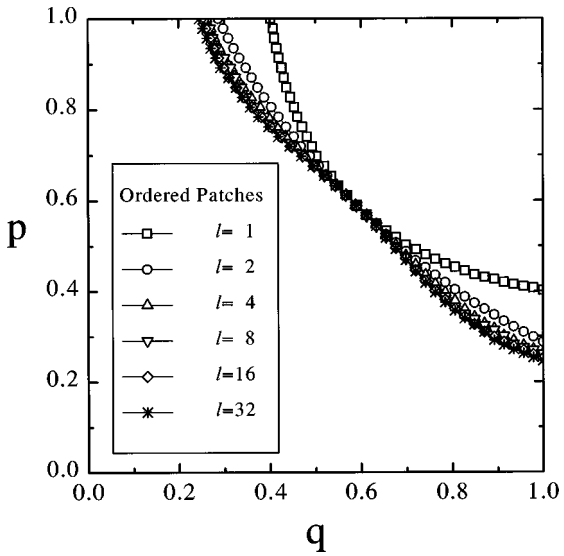

FIG. 1. The phase boundaries for the percolative transition on ordered patchwise lattices, for increasing patches.

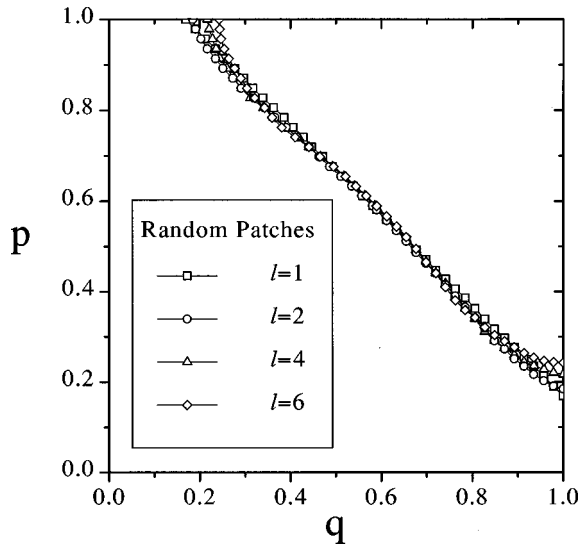

FIG. 2. The same as Fig. 1, but for random patchwise lattices.

From finite-size scaling of percolation it is well known that the thresholds depend on L (see Stauffer and Aharony, Ref. [9]).

Thus, any pair of average thresholds (p_{av},q_{av}) for a lattice of size L and patches with l^2 sites, approaches to the true pair (p_c,q_c) according to the scaling law

$$p_{av}-p_c\sim L^{-1/\nu},\quad q \text{ fixed},$$

$$q_{av}-q_c\sim L^{-1/\nu},\quad p \text{ fixed},\quad l=\text{const}, \tag{1}$$

where ν is the critical exponent of the correlation length ξ, which diverges at any pair (p_c,q_c).

Let Δp and Δq be the root mean-square deviations of the thresholds observed from their average values, i.e.,

$$(\Delta p)^2\equiv\langle(p_{av}-\langle p_{av}\rangle)^2\rangle=\langle p_{av}^2\rangle-\langle p_{av}\rangle^2,$$

$$(\Delta q)^2\equiv\langle(q_{av}-\langle q_{av}\rangle)^2\rangle=\langle q_{av}^2\rangle-\langle q_{av}\rangle^2. \tag{2}$$

But these rms deviations also scale with the system's size [9],

$$\Delta p\sim L^{-1/\nu},\quad \Delta q\sim L^{-1/\nu},\quad l=\text{const}. \tag{3}$$

Then combining Eq. (1) with Eq. (3), we have

$$p_{av}-p_c\sim\Delta p,\quad q_{av}-q_c\sim\Delta q,\quad l=\text{const}. \tag{4}$$

Using the scaling law (1), and taking the universal and exact value $\nu=4/3$, we can find the family of percolation thresholds (p_c,q_c), i.e., for each fixed value of q (or p) we plot the observed thresholds p_{av} (or q_{av}) versus $L^{-1/\nu}$ and then extrapolate to the interception p_c (or q_c) by letting $L\to\infty$. In our calculations, different ratios L/l ($L/l=16$, 24, 36, 48, 64, and 96) were used in order to obtain a good statistical accuracy of the sampling. These simulations were carried out using the Parix parallel computer.

Numerical results, obtained by finite-size scaling for site percolation on ordered and random patchwise lattices, are shown in Figs. 1 and 2, respectively. Note that the critical lines are symmetrical under mirror reflection about the plane $p=q$, since the problem is invariant under the transformation $p\to q$ and $q\to p$. The critical pair $(p_c,q_c)=(0.59,0.59)$ belongs to all transition lines because the site percolation threshold in the square lattice is 0.59.

In ordered lattices we observe that the larger the patch the more spread the percolation zone becomes. More interesting is the behavior in random lattices; enlarging the patches makes the percolation thresholds increase.

In the simplest situation with both sites randomly located $(l=1)$, the transition boundary is the straight line $(p+q)/2=0.59$, i.e., the average concentration is expected to be equal to 0.59 for the full random distribution of sites, like in the classical site percolation.

From many Monte Carlo simulations, series expansions, and a few analytical calculations, is well known that the percolation thresholds depend on both the space dimension d and the coordination number z. Many efforts to find exact relations between these quantities have been made, but with limited success. Very recently, Galam and Mauger have reported universal formulas, which yield within an excellent accuracy both site and bond percolation thresholds, in regular lattices at dimensions $d<7$ [17], and in anisotropic and aperiodic lattices at dimensions $d=2,3$ [18].

We can explain qualitatively these percolative behaviors by means of an effective coordination number. Consider first the evolution of the threshold $q_c^*(l)\equiv q_c(p=1,l)$ corresponding to the pure white site percolation (i.e., all the black sites present), in chessboard lattices, Fig. 1. Clearly, the larger l is, the lower the percolation thresholds $q_c^*(l)$ are. In the case of patches of size $l=1$, any white site has effectively 8 neighbors, Fig. 3(a), and for patches of size $l=2$, a given white site has now 13 connecting neighbors, Fig. 3(b). The effective coordination number for ordered structures with patches of size $l\geqslant 2$ can be easily obtained as follows. Imagine a white square with l^2 sites; then three different types of sites are distinguished, Fig. 3(c): (i) sites at corners, with $z_{co}(l)=6l-1+2(l-1)$ effective neighbors, (ii) sites at edges (excluding sites at corners) with $z_{ed}(l)=3l+(l-1)+1$ effective neighbors, and (iii) centered sites, with only $z_{ce}=4$ neighbors. Since a square with l^2 sites has 4 corner

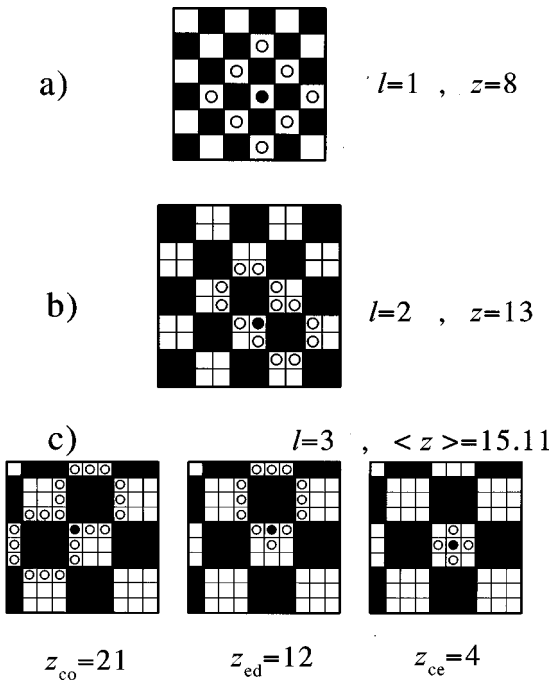

FIG. 3. In a chessboardlike square lattice with all the black squares occupied, $p=1$, any site belonging to a white square has effectively (a) 8 neighbors if $l=1$, (b) 13 neighbors if $l=2$, (c) 15.11 neighbors if $l=3$, and so on, see Eq. (5).

sites, $4(l-2)$ edges sites, and $(l-2)^2$ centered sites, the effective coordination number is

$$\langle z(l)\rangle = \psi_{co}^{(1)}(l)+\psi_{ed}^{(1)}(l)+\psi_{ce}^{(1)}(l)=\frac{4}{l^2}(8l-3) + \frac{4(l-2)}{l^2}(4l)+\frac{4(l-2)^2}{l^2}, \tag{5}$$

being valid for any $l\geqslant 2$.

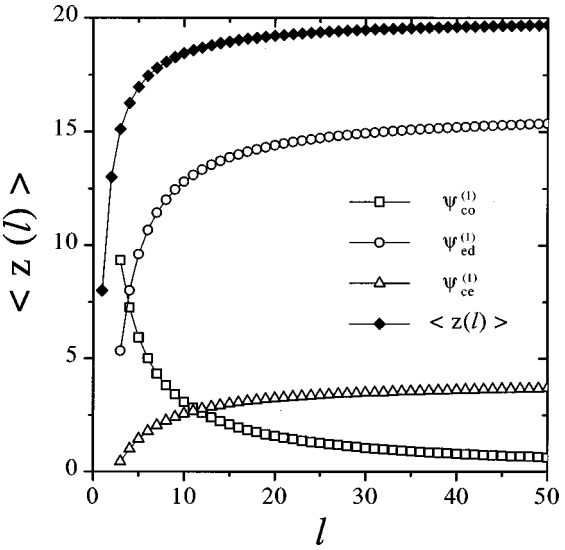

FIG. 4. Evolution of the effective coordination number $\langle z(l)\rangle$ in ordered patchwise lattices, when the dimension l of the patch is increasing. Here, all the black squares are filled ($p=1$).

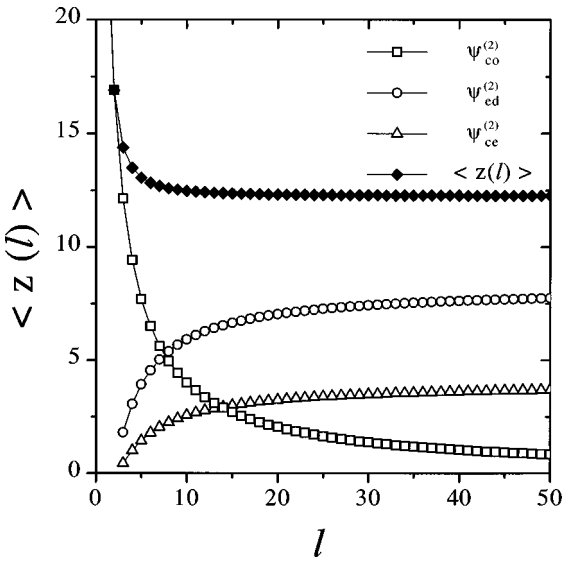

FIG. 5. The same as Fig. 4, but for random patchwise lattices.

The three functions $\psi_{co}^{(1)},\psi_{ed}^{(1)},\psi_{ce}^{(1)}$ and the resulting effective coordination number $\langle z(l)\rangle$ are shown in Fig. 4. Note that the contribution to $\langle z(l)\rangle$ coming from sites at corners vanishes for large l. If $l\to\infty$, $\langle z(l)\rangle$ reaches a maximum value $\langle z_\infty\rangle=20$, which explains why the percolation threshold $q_c^*(l)$ first decreases with l and then saturates to a well defined value ≈ 0.27.

The situation corresponding to $p<1$ is clear: If not all the black sites are filled, the effective coordination number is lower than that given by Eq. (5), and then $q_c(p,l)>q_c^*(l)$.

The same reasoning can be used to understand the percolation properties of random structures. In this case it is evident that the bigger l is, the higher the percolation thresholds $q_c^*(l)$ are, Fig. 2. But for these structures we cannot obtain explicitly an effective coordination number. However, it is even possible to distinguish the same three types of sites, so we can write

$$\langle z(l)\rangle = \psi_{co}^{(2)}(l)+\psi_{ed}^{(2)}(l)+\psi_{ce}^{(2)}(l). \tag{6}$$

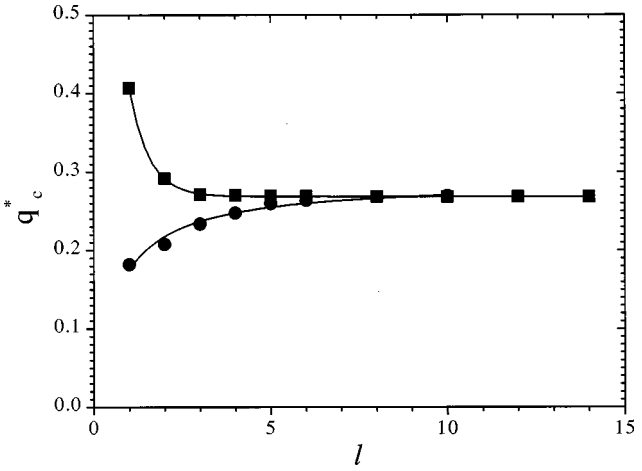

FIG. 6. The percolation threshold q_c^* as a function of l for both the chessboardlike square lattice (circles) and random patchwise lattices (squares).

It is clear that the contribution coming from centered sites is $\psi_{ce}^{(2)}(l)=\psi_{ce}^{(1)}(l)=4(l-2)^2/l^2$, for $l\geqslant 2$.

Numerical results for the functions $\psi_{co}^{(2)}(l)$, $\psi_{ed}^{(2)}(l)$, $\psi_{ce}^{(2)}(l)$ and for the resulting $\langle z(l)\rangle$ are shown in Fig. 5. Note that for small patches the main contribution to $\langle z(l)\rangle$ comes from sites at corners, however, such a contribution vanishes for large l. This fact is due to the presence of large clusters of black sites, which are likely to be very ramified giving a great number of effective connections among white sites. As l increases, the black clusters become less ramified and then the number of perimetrical sites decreases, so their contribution to the effective neighbors also decreases. If $l\rightarrow\infty$, $\langle z(l)\rangle$ goes slowly downwards and reaches a minimum value $\langle z_\infty\rangle\approx 12.5$, which explains why the percolation threshold $q_c^*(l)$ first increases with l and then saturates to a well-defined value ≈ 0.27.

It should be noted that in the limit $l\rightarrow\infty$, the percolation threshold q_c^* in both lattices approaches the value ≈ 0.27, Fig. 6. However, we have shown that their effective coordination numbers are rather different. This is an interesting result and proves that the geometrical distribution of sites is an important property to be taken into account in percolation problems, and here means that percolation is either favored by the random distribution of small patches or by the ordered distribution of large patches. As is expected from percolation theory, in the limit $l\rightarrow\infty$, the transition lines for both lattices coincide in a well-defined and universal critical line since at this limit the percolation problem does not depend on lattice details.

In conclusion, we have presented a simple percolation model in which two types of independent sites are located either in a chessboard structure or in random patches. The results absolutely agree in all limits with well-known results from classical percolation. However, we have shown that transition boundaries are largely affected by the size of the patches as well as by their geometrical distribution.

Future efforts will be addressed to study the relation between conduction and percolation in these structures.

This work was partially supported by CONICET (Argentina) and Fundacion Antorchas (Argentina). The European Economic Community (Project No. ITDC-240) is greatly acknowledged for the provision of valuable equipment. The authors would like to acknowledge stimulating discussions with V.D. Pereyra, J.L. Riccardo, and C. Uebing.

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