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LETTER TO THE EDITOR

Geometrical properties of singly connected bonds in percolation clusters

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Abstract. Numerical simulation of the two-dimensional bond percolation at the percolation threshold on an $L \times L$ lattice shows that the radius of gyration of singly connected bonds (SCB) scales as L^1. This result confirms an assumption used to derive a lower bound on the critical exponent of elasticity. A persistent anisotropy in the distribution of SCB is found and used to estimate the ratio between the bulk and shear moduli of a random percolating system. Local anisotropy in the direction of SCB disappears for large L.

Recently, various aspects of the geometrical properties of percolation clusters on length scales L smaller than the percolation correlation length ξ have received considerable attention. The simple 'nodes and links' model proposed by Skal and Shklovskii (1974) and de Gennes (1976), has been subsequently modified to include the correct scaling of various properties. It was noted by Stanley (1977) that for $L \ll \xi$ the bonds of the infinite cluster can be divided into two groups: singly connected (or cutting, or 'red') bonds (SCB), such that if one is cut the cluster breaks into two parts, and multiply connected (or 'blue') bonds. It was found (Coniglio 1981, Pike and Stanley 1981, Coniglio 1982) that the number of SCB $L_1 \sim L^{1/\nu}$, for $1 \ll L \ll \xi$. Numerous investigations of the geometry of the infinite cluster usually emphasised the various *lengths*, e.g. the scaling of the shortest path between two points (Middlemiss *et al* 1980, Pike and Stanley 1981, Hong and Stanley 1983a, b, Hermann *et al* 1984), as opposed to the *shapes* of various features, since in many problems, such as conductivity or some magnetic phenomena, the connectivity and various lengths (but *not* the shapes) play the major role. Recently, several different Hamiltonians have been used (Kantor and Webman 1984, Bergman and Kantor 1984, Feng and Sen 1984) to describe the elastic properties of random materials. *Vector* displacements of the lattice sites are the variables of these Hamiltonians, and therefore the actual shapes of different paths play an important role in the determination of the effective elastic properties.

In this work I discuss the results of a numerical investigation of several geometrical features of SCB. The results are obtained by Monte Carlo simulation of the bond percolation problem on a two-dimensional (2D) $L \times L$ square lattice at the percolation threshold $p_c = \frac{1}{2}$. The simulations are performed for $2 \leqslant L \leqslant 140$, and the dependence of the various features of SCB on L is checked. The radius of gyration (RMS distance from the centre of mass) of SCB is found to be proportional to L, however there is a persistent anisotropy in the distribution of SCB: the distribution is elongated in the direction of percolation. An estimate of this elongation provides an indication on the universal ratio between the bulk and shear moduli. Local anisotropy in the direction of SCB slowly disappears with increasing L.

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The dependence of an effective elastic constant κ, e.g. bulk modulus or shear modulus, on the volume fraction of a solid component p, near the percolation threshold is given by $\kappa \equiv \kappa_0 (p - p_c)^\tau \sim \xi^{-\tau/\nu}$, where τ is the elastic equivalent of the conductivity exponent t, and ν is the correlation length exponent. On the length scales $1 \ll L \ll \xi$, $\kappa(L) \sim L^{-\tau/\nu}$. The force constant $k(L)$ of an $L \times L$ square (hypercube in d dimensions) can be defined as a ratio of a force applied to its boundary to the average displacement of that boundary, and it is related to the elastic modulus by $\kappa(L) = L^{2-d} k(L)$. If the force constant scales as L^{ζ_E}, then the exponents of the effective elastic modulus and of the force constant can be related by

$$\tau = (d - 2 + \zeta_E)\nu. \tag{1}$$

Kantor and Webman (1984) used an elastic Hamiltonian, which included energy terms proportional to the squares of the changes in the angles between adjacent bonds. For a single chain that Hamiltonian reduces to a very simple form, which is analytically solvable. It can be shown that the force constant of such a chain is

$$k \sim S_\perp^{-2} N^{-1}, \tag{2}$$

where N is the length of the chain and $S_\perp$ is the radius of gyration in the direction perpendicular to the applied force.

This result can be used to obtain bounds on ζ_E (or τ). If we assume that in the actual percolation problem all the multiply connected bonds are infinitely rigid then we can obtain the upper bound on k and, thus, the lower bound on ζ_E. Replacing N in (2) by $L_1 \sim L^{1/\nu}$, and $S_\perp$ by L^α, where the exponent α describes the divergence of the radius of gyration of the SCB with L, and using the definition of ζ_E, we obtain $\zeta_E \geqslant 2\alpha + 1/\nu$. Kantor and Webman (1984) assumed that SCB are homogeneously distributed, i.e. $\alpha = 1$, and arrived at the bound $\zeta_E \geqslant 2 + 1/\nu$. This assumption is confirmed here by numerical simulation. Similar arguments can be used to obtain an upper bound on ζ_E. If we neglect all the bonds except those contained in the shortest path between two points, the length of which diverges as L^z, then we underestimate k and overestimate ζ_E. Thus the bounds on τ are:

$$d\nu + 1 \leqslant \tau \leqslant (d + z)\nu. \tag{3}$$

Using the known values of ν (see, e.g., Stauffer 1980) and the values of z obtained by Hermann *et al* (1984) we find that $3.7 \leqslant \tau \leqslant 4.2$ in 2D, and $3.6 \leqslant \tau \leqslant 3.8$ in 3D. (The uncertainties in the numerical values of the bounds are smaller than 0.1 and are caused by the uncertainties in the numerical values of ν and z.) For $d = 6$ both bounds coincide and give $\tau = 4$. Numerical simulation of a 2D system (Bergman 1984) gives $\tau = 3.5 \pm 0.2$, while a 'table-top' experiment (Benguigui 1984) estimates $\tau = 3.5 \pm 0.4$. Although these results are reasonably consistent with the lower bound on τ, they raise a certain suspicion on the assumption $\alpha = 1$.

Generally, SCB can be defined as follows: We chose two boundary sets of points, A and B, on a finite geometrical figure, such as a percolation cluster. A bond is called 'singly connected' if its removal leaves no continuous path between at least one point of the set A and a point of the set B. Although it is numerically convenient to choose each set to contain only one point (e.g., Pike and Stanley 1981), a different choice, where the two boundary sets represent two opposite edges of a square (faces of a hypercube) is more directly related (Coniglio 1982) to the position-space renormalisation group approach (see, e.g., Reynolds *et al* 1980). Although the point-to-point and the edge-to-edge definitions of SCB give different results for the same L, the scaling

powers are the same in both definitions. In the present simulation I used the edge-to-edge definition of SCB, and the following procedure: (1) 24 000 bond percolation configurations at p_c have been created on an $L \times L$ square lattice for each value of L ($2 \leqslant L \leqslant 140$). (2) Each configuration was tested to determine whether it contained a continuous path between $x = 0$ and $x = L$ edges, i.e. percolated in y direction, and only the percolating configurations (half of all the configurations) have been considered. (3) In each percolating configuration the number L_1 of SCB, the number L_{1x} of SCB which point in x direction, the squared radius of gyration S^2 of SCB and the squared radius of gyration S_x^2 of the x coordinate of SCB have been calculated. (4) Those quantities have been averaged over 12 000 configurations. The standard deviation of each of those quantities (for fixed L) is comparable to its mean value, and the averaging over the large amount of configurations reduces the standard deviation of the average to a few percent of the average.

The upper line in figure 1 depicts the dependence of L_1 on L. The inverse slope of this line is $\nu = 1.35 \pm 0.02$ in good agreement with the known value of this exponent (Reynolds *et al* 1980). The remaining two curves in figure 1 depict S and S_x as functions of L. Both curves have asymptotic slope $\alpha = 0.97 \pm 0.03$. This result is consistent with the assumption $\alpha = 1$, which can be obtained from the following considerations: If the point-to-point definition of SCB is used then it is clear that the density of SCB near the boundary points must be at least as high as their density between the points, and therefore, at least the radius of gyration of the component along the straight line connecting the two boundary points must scale as L. In the case of the edge-to-edge definition of SCB the situation is reversed, namely the density of SCB in the middle of the square will be higher than their density near the edges (or at least as high). However, if the radius of gyration is related to the physical properties of the system it should scale as L also in this case.

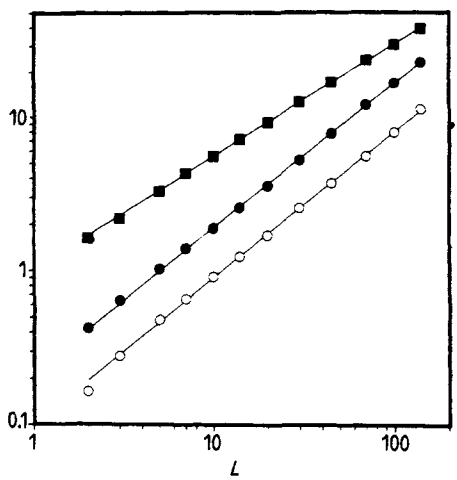

Figure 1. Double logarithmic plot showing the relationship between the number of SCB L_1 (■), their radius of gyration S (●), the radius of gyration S_x of their x coordinate (○) and the size of the lattice L. The standard deviation of the average of L_1 is ~1.5% (the symbol is four times larger than the error bars), and for S and S_x it is 3% (the symbol is twice as large as the error bars).

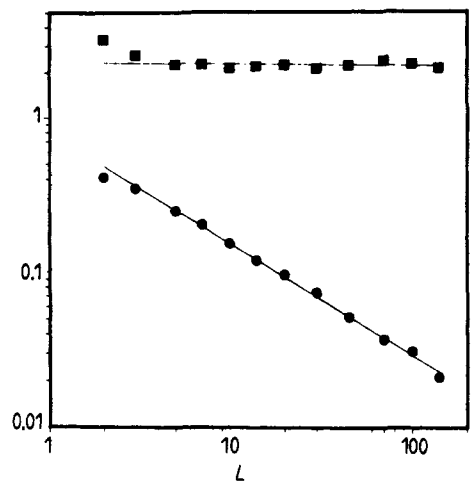

Figure 2. Double logarithmic plot showing the ratio $S^2/2S_x^2$ (■), and $1/2 - L_{1x}/L_1$ (●) as a function of lattice size L. The statistical error of $S^2/2S_x^2$ is ~6% (the size of the symbol), and the errors in the second curve are less than 2% (the symbol is six or more times larger than the error bars).

The above arguments do not apply to the radius of gyration S_x of the coordinate perpendicular to the direction of percolation. Note, that the isotropy arguments do not apply in this case: If instead of percolation in y direction we would consider percolation in x direction, there would be a *different* set of SCB even for the same percolation cluster. Although a different behaviour of S_x and S_y cannot be excluded by isotropy arguments, it is reasonable to expect both of them to scale, at least, with the same power. The bottom curve in figure 1 confirms this expectation. For an isotropic case we would expect $S^2/2S_x^2$ (or S_y^2/S_x^2) to approach 1 for sufficiently large L. The upper curve in figure 2 shows that the ratio apparently approaches the value 2.2 ± 0.1 (or $S_y^2/S_x^2 = 3.4 \pm 0.2$), i.e. the distribution of SCB is elongated in the direction of percolation. This is a universal ratio, i.e. it is independent of the particular choice of the lattice type. This feature somewhat reminds the anisotropy of the unrestricted (Koyama 1967, 1968, Šoltz and Stockmayer 1971, Šoltz 1971) and self-repelling (Mazur *et al* 1973, Rubin and Mazur 1977) random walks. However, the 'long dimension' in our case is predetermined by the choice of the direction of percolation, while the anisotropy of the random walks is 'spontaneously' generated and has a random orientation. From (2) we find that $S_y^2/S_x^2 = k_y/k_x$, where k_x and k_y are the force constants for forces applied in x and y directions, respectively, in the model which assumed that all multiply connected bonds are infinitely rigid. This result can be interpreted as the ratio between the upper bound on the component of the elastic stiffness tensor $C_{1111} = \kappa + \mu$ (κ and μ are the 2D bulk and shear moduli, respectively) and the upper bound on μ. Although this is only a ratio of the upper bounds on those quantities, it surprisingly agrees with the result 3.5 ± 0.2 of the numerical simulation (Bergman 1984) of the actual percolation problem, and is close to the value 3 predicted from the solution of an elastic Sierpinski gasket and the analysis of the Clausius–Mossotti and the effective medium approximations (Bergman and Kantor 1984).

Finally, we checked the ratio of the number L_{1x} of SCB which point in x direction to the total number L_1 of SCB. For small L, L_{1x} is, obviously, a small portion of L_1. However, we expect the ratio to approach the value $\frac{1}{2}$ for $L \to \infty$, i.e. the local lattice dependent geometry should not reflect the direction of the percolation. Since this anisotropy has nothing to do with the critical properties of SCB and is only related to the anisotropic boundary conditions ($L_{1x} = 0$, for $L = 1$) we can expect it to disappear in a simple form: $L_{1y}(L) \cong L_{1x}(L) + \text{constant}$, for $L \to \infty$, or $(\frac{1}{2} - L_{1x}/L_1) \sim L_1^{-1} \sim L^{-1/\nu}$. This behaviour is depicted by the lower curve of figure 2. The inverse slope is -1.36 ± 0.04 in good agreement with the value of ν which has been obtained previously. Note, that the prefactor of the power law is ~ 1, and therefore even for $L \simeq 40$ the number of x-directed bonds is still by 15% smaller than the number of y-directed bonds. While this anisotropy is completely irrelevant for conductivity measurements, it has some importance in the studies of elasticity. This result indicates that in Monte Carlo simulations of elasticity larger L's will be needed than in conductivity measurements to attain the same accuracy.

In this work, scaling behaviour of several geometrical properties of SCB has been investigated, and it was shown that the knowledge of these properties can be useful in the investigation of certain physical properties of the system. Further investigations of those properties (especially the ratio S_y^2/S_x^2) on larger and different kinds of lattices would be useful. In six dimensions, where the number of the SCB, the length of the shortest path between two points and the random walks have the same scaling behaviour, an investigation of the anisotropy of those objects could provide an insight into its nature.

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