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LETTER TO THE EDITOR

The chemical distance distribution in percolation clusters

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Abstract. We study the conditional probability density $p(r|l)$, for the geometrical distance r corresponding to a given chemical distance l for percolation clusters in two dimensions. We argue that (i) $p(r|l) = A_l x^{\tilde{g}} \exp(-ax^{\tilde{\delta}})$ where $x = r/l^{\tilde{\nu}}$, $\tilde{g} = 2.5 \pm 0.3$, $\tilde{\delta} = 9.8 \pm 0.5$, and $\tilde{\nu} = 0.88 \pm 0.02$, and (ii) there is a relation $\tilde{\delta} = (1 - \tilde{\nu})^{-1}$ which is in good agreement with our numerical data. These results are derived by considering a special class of self-avoiding walks consisting of chains which are chemical paths (shortest paths) on critical percolation clusters.

There has been considerable interest recently in the intrinsic properties of random aggregates (Alexandrowicz 1980, Middlemis *et al* 1980, Pike and Stanley 1981, Alexander and Orbach 1982, Havlin and Nossal 1984, Herrmann *et al* 1984, Ritzenberg and Cohen 1984, Vannimenus *et al* 1984). Two natural measures of distance are usually used to characterise a fractal (Mandelbrot 1982). These are the geometrical distance, r, and the so-called intrinsic chemical distance, l, defined as the shortest distance measured along the fractal structure between two sites. Exponents related to the chemical distance are found to be useful in characterising the dynamics of random aggregates (Havlin *et al* 1984, Witten and Kantor 1984). In this letter we suggest a form for the conditional probability density $p(r|l)$, for the geometric distance r corresponding to a given chemical distance l, for percolation clusters. Practically, we discuss the ensemble of self-avoiding walks (SAWs) defined by the shortest paths (i.e., chemical distance) between any two sites on the incipient infinite percolation clusters (Stauffer 1979) similar to the elastic backbones (Herrmann *et al* 1984). Thus $p(r|l)$ is the probability of obtaining an l-steps SAW with an end-to-end length r in such an ensemble. Further results are presented for the expected elongation of these chains in the presence of a stretching force.

The conditional probability density, $p(r|l)$, was determined numerically for percolation clusters generated on a 2D triangular lattice using a growth method suggested by Alexandrowicz (1980). The estimate of $p(r|l)$ was obtained, by enumerating the geometric distances between points at fixed values of the chemical distance and normalising the results. In order to present our results we require the exponent, which relates the average geometrical distance between sites which are separated by a chemical distance l by

$$\bar{r} \sim l^{\tilde{\nu}}. \tag{1}$$

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The exponent $\tilde{\nu}$ can be related to the way the mass of a fractal scales with r and l. The mass, M, scales with r as $M \sim r^{d_f}$ where d_f is the fractal dimension, and with l as $M \sim l^{d_l}$. Consequently $\tilde{\nu}$ can also be expressed as

$$\tilde{\nu} = d_l / d_f. \tag{2}$$

Our data for $l = 50$, 100, 150, and 200 are summarised in figure 1. They indicate that $p(r|l)l^{\tilde{\nu}}$ can be written in terms of a single scaled coordinate $x = r/l^{\tilde{\nu}}$, where $\tilde{\nu} = 0.88$. The form of $p(r|l)$ suggested by an argument used in the theory of SAWs is (deGennes 1979, Domb 1969, McKenzie 1976, Fisher 1966, Fisher and Burford 1967)

$$P(r|l) = A_l f(x) = A_l x^{\tilde{g}} \exp(-a x^{\tilde{\delta}}) \tag{3}$$

where a is a constant. The normalisation of $p(r|l)$ has the consequence that $A = A_0/l^{\tilde{\nu}}$ where A_0 is independent of r and l. The scaling behaviour indicated in figure 1 is best fit by the values $\tilde{g} = 2.5 \pm 0.3$ and $\tilde{\delta} = 9.8 \pm 0.5$ and the result agrees very well with our simulated data, see figure 1. (The ± values were determined by varying the values of $\tilde{g}$ and $\tilde{\delta}$ and retaining only those values that gave a satisfactory fit by eye.) We emphasise the fact that $p(r|l)$ is a distribution function describing both a property of percolation *clusters* as well as the ensemble of a special class of SAWs, i.e., the chains obtained from the chemical paths connecting any two sites on a critical percolation cluster disregarding all of the remaining sites.

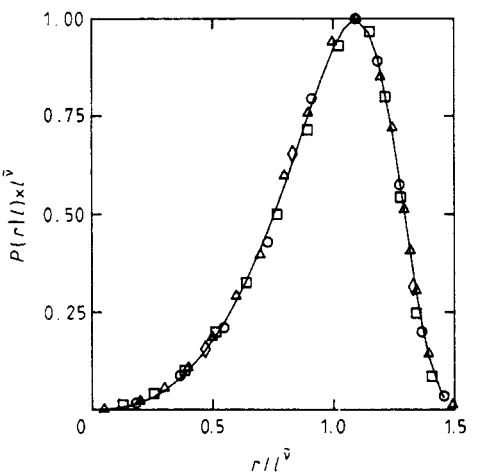

Figure 1. The conditional probability density $p(r|l)$ for the geometrical distance r corresponding to a given chemical distance l. The different signs represent different chemical distances; $l = 50$ (◇), $l = 100$ (○), $l = 150$ (□), $l = 200$ (△). The full line represents the best fit, equation (3).

In order to study the implications of (3), let us consider a stretching force, f, applied on a chain of chemical distance l. The partition function can be written (see e.g., de Gennes 1979)

$$Z(l) = \int P(r|l) \exp(-\beta f r)\, \mathrm{d}r \tag{4}$$

which is a function of the constant force f and the chemical distance l. The average

elongation is given by

$$\langle \Delta r \rangle = -\partial \ln Z(l)/\partial \ln(\beta f). \tag{5}$$

When f is large, the form of $p(r|l)$ can be substituted into (4), and the resulting integral evaluated asymptotically. The result of this calculation is

$$\langle \Delta r \rangle = f^{1/(\tilde{\delta}-1)} l^{\tilde{\nu}\tilde{\delta}/(\tilde{\delta}-1)}. \tag{6}$$

Using the assumption (de Gennes 1979 and references cited therein) that $\langle \Delta r \rangle$ scales linearly with l at large values of f it follows that

$$\tilde{\delta} = (1-\tilde{\nu})^{-1} \tag{7}$$

which is similar to the known relation between δ and ν in ordinary SAWs (de Gennes 1979, Fisher 1966, Fisher and Burford 1967, Domb 1969, McKenzie 1976, Pincus 1976). This result is in good agreement with the estimated values $\tilde{\delta} = 9.8 \pm 0.5$, $\tilde{\nu} = 0.88 \pm 0.02$.

To summarise, in spite of the fact that $\tilde{\delta}$ and $\tilde{\nu}$ describe percolation clusters, they describe also a special class of SAWs. These are SAWs with a step-step interaction governed by the percolation cluster's constraints. The SAWs are more swelled than ordinary SAWs, and in fact their upper critical dimensionality is $d_c = 6$ (compared to $d_c = 4$ for regular SAWs). We have exploited SAWs theory to derive the relation between the two percolation exponents $\tilde{\nu}$ and $\tilde{\delta}$ (7). It should be noted that (7) is also valid for the lattice animal model of branch polymers. Since it was found recently (Havlin *et al* 1984) that $\tilde{\nu} = 0.85$, 0.74, 0.67 and 0.5 for lattice animals in $d = 2$, 3, 4 and 8 dimensions respectively we expect $\tilde{\delta} = 6.9$, 3.8, 3.0 and 2 for these dimensions. In the case of percolation clusters (7) is exactly valid for $d = 1$ where $p(r|l)$ is a delta function as well as for $d \geqslant 6$ where it is accepted that $p(r|l)$ becomes a Gaussian; $\tilde{\delta} = 2$ (de Gennes 1979). It would be interesting to study $p(r|l)$ in $d = 3$ for which $\tilde{\nu} = 0.74 \pm 0.3$ In this case the prediction of (7) is $\tilde{\delta} = 4$. It would also be of interest to find any relation between $\tilde{g}$ and other percolation exponents.

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