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LETTER TO THE EDITOR

Ideal chain on a two-dimensional critical percolation cluster

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Abstract. We study the statistics of the *ideal chain* (or equally weighted trajectories) for the first time on a two-dimensional critical percolation cluster. We discuss the asymptotic behaviour of the mean end-to-end distance and the number of chains for the long chain limit by exact enumeration. Our results strongly suggest that this problem does not belong to the same universality class as the *random walk* (or kinetically weighted trajectories) on the same fractal cluster.

Random walks (RW) have been studied extensively on (Euclidean) hypercubic lattices [1], on (deterministic) self-similar structures (*exact* fractals) [2], and also on disordered systems (e.g. [2, 3] and references therein). This problem is intimately related to another problem called the ideal chain (IC), which models the polymers in solution in the limit of no excluded volume effects [4]. Unlike the RW, the statistical weight given at each step for the IC is a constant independent of the connectivity of the location of the monomer (represented by the coordination number on a lattice). As a consequence, the total statistical weight of a chain does not depend on the type of sites visited but only on the length of the chain itself. A way to picture this is to think of the RW as a dynamical problem and of the IC as a static one [5].

Although the two problems are certainly equivalent on Euclidean lattices with all sites having the same corrdination number, they have been shown to differ on specific examples of exact fractals [6]. In certain exact fractals where the sites of the highest coordination number do not form an infinite connected network, the asymptotic long chain behaviour was found to be *localized*, such as $R \sim e^{\sqrt{\log N}}$ or $R \sim (\log N)^x$ $(x > 0)$ [6] where R is the mean linear size and N is the contour length of the chain. Since the ideal chain tends to visit the sites with high coordination numbers preferentially, it is plausible that the chain is less swollen if those sites tend not to be a part of the extended network.

On the other hand, in some cases where the sites of the highest coordination number are part of the infinite connected network, a power-law behaviour for the mean end-to-end distance was found. However, even in such cases, the value of the Flory exponent ν [4] was significantly different (always higher) than the corresponding one for the random walk problem on the same structure [6]. In all the cases previously studied, the behaviour of the asymptotic number of chains (or the *entropy*) was found to be qualitatively the same as the RW problem, possibly with different values of the corresponding exponents.

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Subsequent numerical work [7] also showed that on some more complicated fractal structures, such as certain deterministic fractal *surfaces*, this was not the case. In those cases, a power-law behaviour for the IC was found with an exponent very close to that for the RW.

It is then very interesting to ask whether or not this kind of difference in behaviours between IC and RW exists in statistical (or *disordered*) fractals. In the present work, our aim is to investigate the IC problem on a two-dimensional lattice with quenched forbidden regions which occur stochastically. A simple model of such a system is the percolation cluster [8]. Let p be the independent probability that a given site is occupied (and thus available to the chain). At the percolation threshold p_c, the critical cluster formed by connecting occupied nearest-neighbour sites can be considered self-similar at all scales (since the correlation length is infinite) (see e.g. [8]). This is therefore a very handy example of a statistical fractal for our purpose. We are aware that there was a previous study of this problem by a different approach in an unpublished work by Vanderzande [9].

We numerically generate such a critical percolation cluster from a seed site on a square lattice using a computer algorithm which falls in the category of the breadth-first search (see e.g. [3]). The clusters used in this work are obtained in this way up to the 300th generation (or *chemical distance* [2] equal to 300). All the ICs of a given (contour) length that start from selected occupied sites are then enumerated exactly and their properties, particularly the end-to-end distances and how many chains there are, are investigated.

Let c be a given chain starting from site $\boldsymbol{P}$ of the cluster $\mathscr{C}$ at the percolation threshold p_c. We define $\mathscr{C}$ relative to the seed site; thus even an identically shaped cluster would be considered distinct if it is displaced from $\mathscr{C}$ relative to the seed $\mathbf{0}$. Then the number $C(N, \boldsymbol{P})$ of N-step chains starting from $\boldsymbol{P}$ and terminating anywhere in the cluster is:

$$C(N, \boldsymbol{P}) = \sum_{c \in \mathscr{C}} 1. \tag{1}$$

Another quantity of interest is the mean square end-to-end distance $\langle R_N^2 \rangle$ of N-step chains $c \in \mathscr{C}$ defined as:

$$\langle R_N^2 \rangle = \frac{\Sigma_{c \in \mathscr{C}} \mathscr{P}(c) R_N^2(c)}{\Sigma_{c \in \mathscr{C}} \mathscr{P}(c)}. \tag{2}$$

As mentioned above the weight $\mathscr{P}(c)$ given to the chain c is a constant independent of its environment and depends only upon the length of the chain. Clearly this factor cancels out both from the numerator and denominator, leaving the number of chains in the denominator. This is indeed what one gets from the usual self-avoiding walk (SAW) problem if the constraint of self-avoidance is released. In this sense, the usual SAW problem should also be called the self-avoiding chain.

The difference from the usual random walk is that in the latter the weight $\mathscr{P}(w)$ given to a walk w is a function of the visited sites which depends upon the model chosen. For example in the case of the *myopic ant* [10], $\mathscr{P}(w) = \Pi_{i \in \mathscr{C}} 1/z_i$ where z_i is the coordination number of the ith site visited by the walk. In the case of the *blind ant* the probability to hop to a particular nearest-neighbour site is a constant independent of the current location. However, there is a finite probability for the blind ant to stay at the current site if some of the neighbours are unoccupied. It is this probability which makes this problem different from the IC.

The final average is the *quenched* average over all the possible disorder configurations $\mathscr{C}$ defined as

$$\overline{f(\mathscr{C})} = \sum_{\mathscr{C}} P(\mathscr{C}) f(\mathscr{C}) \tag{3}$$

for any property $f(\mathscr{C})$ of the configuration $\mathscr{C}$ where $P(\mathscr{C})$ is the probability of occurrence of $\mathscr{C}$. We generally indicate the disorder average by a bar above the quantity.

We could also consider averaging over the starting points of the chains or walks:

$$\hat{C}(N) = \frac{\Sigma_r C(N, r)}{|\mathscr{C}|} \tag{4}$$

where $|\mathscr{C}|$ is the number of sites in the cluster $\mathscr{C}$. A similar definition can be given also for $\langle R_N^2 \rangle$. Since any cluster looks different when viewed from different sites, this last average can be regarded as sort of a disorder average even though it is for a given cluster $\mathscr{C}$. Averages over starting points on a given configuration will be denoted by a hat above the quantity.

The averaged quantities defined above are assumed to have asymptotic power-law dependence on N. This assumption is, of course, to be tested *a posteriori*. Thus we assume, in the limit of $N \gg 1$,

$$\overline{C(N, \mathbf{0})} \sim \mu^N N^{\gamma - 1} \tag{5}$$

$$\overline{\langle R_N^2 \rangle} \sim N^{2\nu} \tag{6}$$

and investigate whether good fits can be obtained for suitable values of the exponents γ and ν as well as for the effective coordination number μ.

If $S = |\mathscr{C}|$ is the total number of sites in a given cluster $\mathscr{C}$, the connectivity of the percolating cluster is stored in an $S \times S$ matrix $\mathbf{W}_{ij}$ such that $\mathbf{W}_{ij} = 1$ if sites i and j are nearest neighbours and $i, j \in \mathscr{C}$, and 0 otherwise. Let us further define two vectors of S components: $\boldsymbol{a}$ where $a_1 = 1$ and $a_j = 0$ for $j = 2, \ldots, S$, and $\boldsymbol{b}$ where $b_j = 1$ for $j = 1, 2, \ldots, S$, where we denote the seed site $\mathbf{0}$ by $i = 1$. Then

$$C_N \equiv C(N, \mathbf{0}) = \sum_{i,j} b_i (\boldsymbol{W}^N)_{ij} a_j \tag{7}$$

for each configuration $\mathscr{C}$.

In a similar way we can calculate the mean square end-to-end distance $\langle R_N^2 \rangle = \langle (\boldsymbol{r}_N - \boldsymbol{r}_0)^2 \rangle$, where $\boldsymbol{r}_N$ is the end position of the Nth step and $\boldsymbol{r}_0$ is that of $\mathbf{0}$. It is easy to see that, if we define a vector $\mathscr{R}$ of S components by $\mathscr{R}_1 = 0$ and $\mathscr{R}_j = (\boldsymbol{r}(j) - \boldsymbol{r}_0)^2$ for $j = 2, 3, \ldots$ where $\boldsymbol{r}(j)$ is the coordinates of the jth site on the cluster, then we have

$$\langle R_N^2 \rangle = \frac{\Sigma_{i,j} \mathscr{R}_i (\mathbf{W}^N)_{ij} a_j}{\Sigma_{i,j} b_i (\mathbf{W}^N)_{ij} a_j}. \tag{8}$$

In order to avoid an overflow which would otherwise quickly occur in the numerical computation of these quantities, we use a suitable Gram–Schmidt normalization procedure by which the result of the multiplication by $\mathbf{W}$ is normalized at every step. It is also worth mentioning that apart from the generation of the percolation cluster, the calculations of the various quantities are exact.

The results are shown in figure 1 for a maximum number of steps of 1600 averaged over 1000 different clusters. These clusters were generated to the chemical distance 300 and had a mean size of about 12 300 and a standard deviation of about 4800. The mean square end-to-end distance exponent 2ν is computed by means of a linear

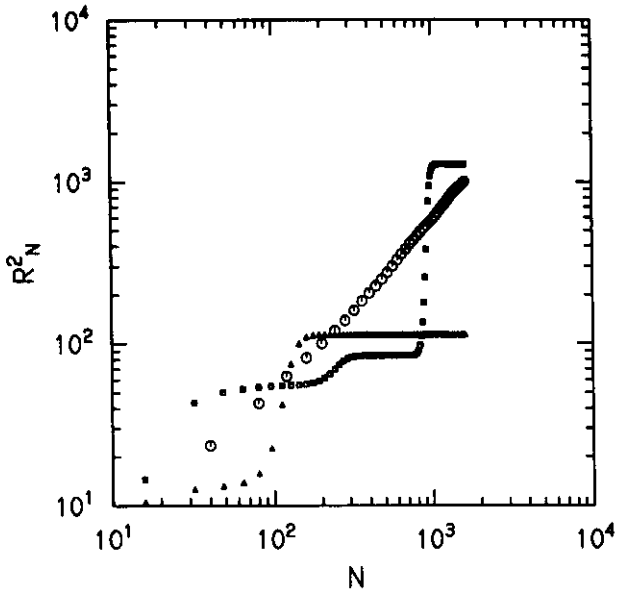

Figure 1. Log–log plot of the mean square end-to-end distance $\overline{\langle R_N^2 \rangle}$ averaged over disorder (○) and results from two individual clusters (□, △).

least-squares fit to the log–log plot of $\log\overline{\langle R_N^2 \rangle}$ against $\log N$, which yields a value 1.1616 ± 0.022. This estimate was obtained by first calculating the average over 3 batches of 1000 clusters each for each selected value of N and then performing a linear regression on these values in the log–log scale. The error estimate is the standard regression error. This estimate has been checked for a possible N dependence of the slope by calculating an *effective* N-dependent exponent ν_N by the same method as was used in the context of the self-avoiding walk problem [11] and then extrapolating it to $N \to \infty$. The result is in agreement with the quote estimate (cf figure 2).

This value of ν would correspond to the associated fractal dimension of the chain $d_c = 1/\nu \approx 1.7$, whereas the best known estimate for the RW problem on the critical percolation cluster is in the range 2.8–2.9 [3]. This result is consistent with the previous analysis [6] for some exact fractals where the sites of the highest coordination number do form an infinite connected cluster.

Also shown in figure 1 are some typical results for $\langle R_N^2 \rangle$ for individual clusters. Clearly, chain dimensions increase as a function of the number of steps N in discrete steps followed by flat plateaux, and the disorder average removes this discrete structure resulting in the smooth final curve. (It may be worth mentioning that the large local slope where the jumps take place does *not* imply larger than linear extension.) This behaviour indicates that the ideal chain does not visit the cluster uniformly, but tends to move from a localized region to another in discrete jumps. The obvious suggestion is that these localized regions correspond to areas of high connectivity and the step structure thus reflects the cluster topology. We also checked that such a feature is *not* present in the case of the random walk (both for the blind and the myopic ant) where the diffusion for a fixed cluster follows a power law and the average simply picks out the best slope. This aspect of the problem is presently being investigated and the results will be reported subsequently.

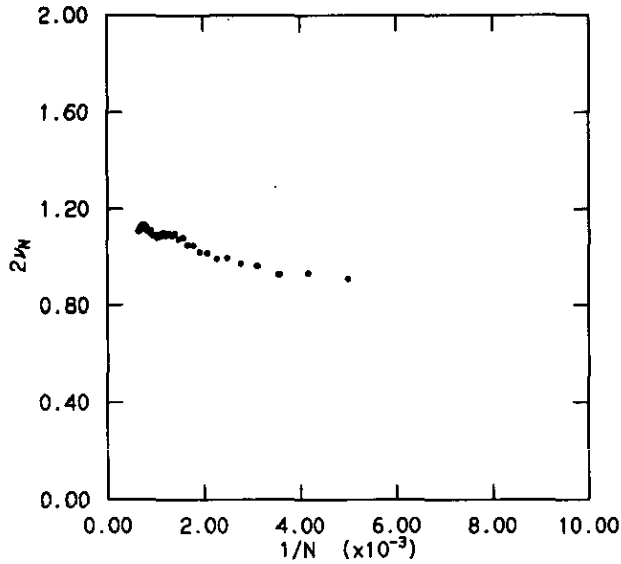

Figure 2. Effective exponent ν_N calculated using the recipe given in [11] is given against $1/N$.

If we instead average over 1000 starting points randomly chosen on a given cluster, we obtain quite similar results (not shown). Again the step structure of the results from individual starting points disappears as the average is taken over the starting points.

In view of the non-uniform behaviour of the ideal chain, we also checked for the possibility of multifractal scaling for the moments of the end-to-end distance R. We first performed an analysis of the probability $P(R)$ of finding the chain at a distance $R = |r_N - r_0|$ from the starting point, and plot the quantity $P(R)N^{\nu}$ against R/N^{ν} for different values of N in figure 3. The result is clearly consistent with simple scaling. In figure 4 we also show the different moments $q = 0$, 0.5, 1, 1.5, 2 of the quantity $\langle R_N^q \rangle^{1/q}$. We report the corresponding numerical estimates of the exponent ν and the effective coordination number μ in table 1. The result shows an increasing trend (although gradual) of the estimate of $\nu(q)$ as q increases. Thus the scaling of the probability $P(R)$ is not perfect and there is the possibility of a multifractal distribution. This may be related to the *staircase* behaviour for the size of the ideal chains, whereby different moments emphasize correspondingly different scales. Further work on this point is in progress.

In the case of the RW it is known that the constraint of the conservation of the probability gives $\gamma = 1$.

It is not however obvious that the same value is to be found for the IC problem. Indeed in some cases of the deterministic fractals considered in [6], it was found that this was not actually true. Nevertheless, our results strongly indicate that the value for γ is 1. This can be inferred by looking at the quantity:

$$\log\left(\frac{\overline{C_{N+\Delta N}}}{\overline{C_N}}\right) \approx \log \mu + (\gamma - 1)\frac{\Delta N}{N} \tag{9}$$

against $\Delta N/N$, where the flat trend as $N \to \infty$ corresponds to $\gamma = 1$.

By means of a linear fit of the quantity $\log \overline{C_N}$ against $\log N$, one can also obtain the value of μ, the effective coordination number. The disorder average of this value

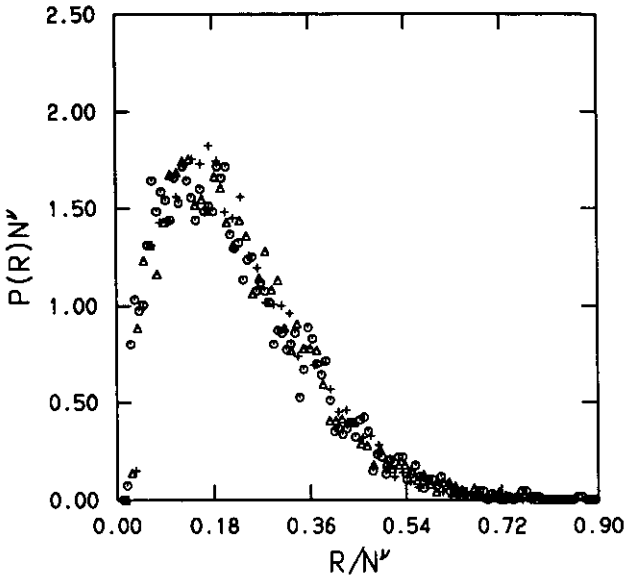

Figure 3. Scaled probability distribution $P(N)N^{\nu}$ against scaled end-to-end distance R/N^{ν}, for $N = 520(+), 800(\triangle), 1600(\bigcirc)$. The value of ν used for scaling is $\nu = 0.56$.

is $\mu = 3.567 \pm 0.001$, where the estimates are obtained in the same way as for R_N^2. This estimate is much higher than the typical value found in the RW case, as expected.

It is also interesting to look at the different moments of the number of walks. In figure 5 we show the quantity $C_N^{q\,1/q}$ for $q = 0, 0.5, 1, 1.5, 2$. (It may be worth mentioning that the $q = 1$ moment is not trivially related to C_N for the fully occupied lattice unlike for the SAW problem on disordered clusters.) The corresponding numerical estimates

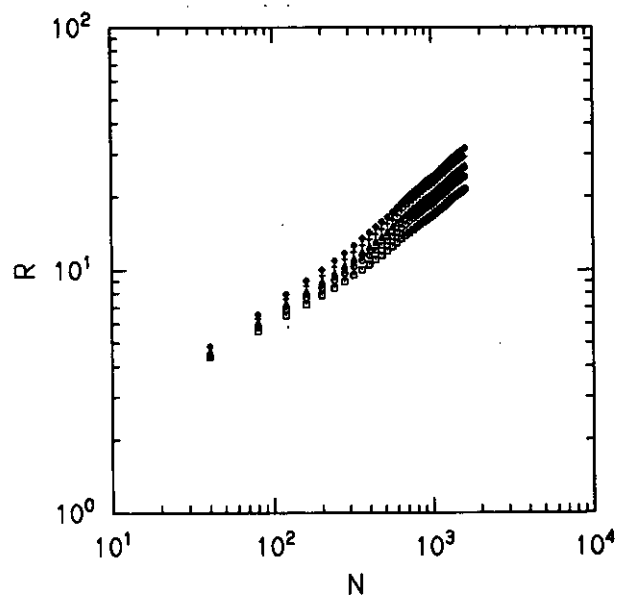

Figure 4. Log–log plot of the moments $R \equiv \overline{\langle R_N^q \rangle}^{1/q}$ for the values $q = 0(\square), 0.5(\bigcirc), 1(\triangle), 1.5(+), 2.0(\diamond)$.

Table 1. Moments for $\overline{\langle R_N^q \rangle}^{1/q} \sim N^{\nu(q)}$.

q	0	0.5	1	1.5	2
ν	0.517 ± 0.013	0.541 ± 0.011	0.558 ± 0.011	0.571 ± 0.011	0.580 ± 0.011

for μ are given in table 2. They show a different behaviour for the $q = 0$ (i.e. logarithmic) moment compared with all the other moments. Since the $q = 0$ moment corresponds to the most probable value [12], this difference reflects the fact that the IC is a random multiplicative process unlike the RW.

When the average over all starting points is performed before the average over all clusters, we get a much faster convergence for the quantity $\bar{\gamma}$. This is expected since, according to the previous argument, this is equivalent to taking an average over a much larger number of disorder configurations. In this way, we also find the effective coordination $\bar{\mu}$ to be $\bar{\mu} = 3.681 \pm 0.001$.

The asymptotic behaviour of the many quantities can be obtained from the spectral properties of the sparse matrix **W** [13]. On this basis, we are conducting a detailed investigation of these properties. The basic result appears to be that the density of the eigenvalues do not increase appreciably in the neighbourhood of the maximum eigenvalue. Physically this would mean that only the maximum eigenvalue matters for the

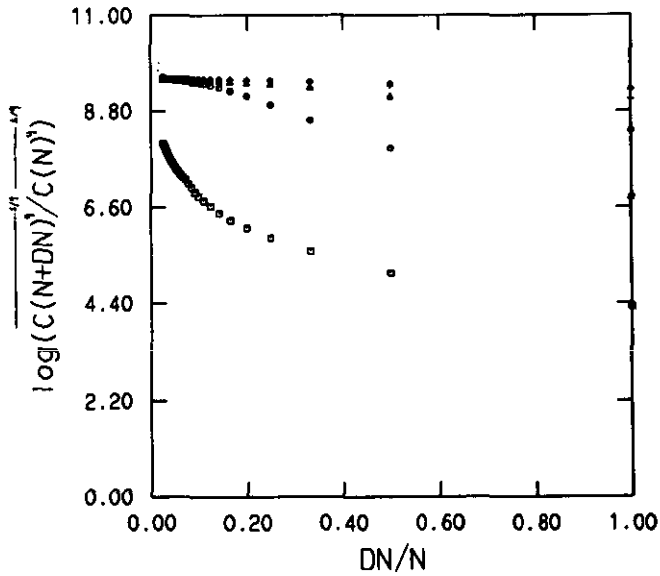

Figure 5. Plot of the quantity $\log(\overline{C_{N+\Delta N}^q}^{1/q} / \overline{C_N^q}^{1/q})$ against $\Delta N/N$, for the moments $q = 0(\square)$, $0.5(\bigcirc)$, $1.0(\triangle)$, $1.5(+)$, $2.0(\diamond)$. The result shows the different behaviour of the $q = 0$ (or logarithmic) moment with respect to the others.

Table 2. Moments for $\overline{C_N^q}^{1/q} \sim \mu(q)^N N^{\gamma(q)-1}$.

q	0	0.5	1	1.5	2
μ	3.353 ± 0.001	3.558 ± 0.002	3.567 ± 0.002	3.569 ± 0.002	3.569 ± 0.002

asymptotic large N behaviour. Thus, we may expect $\overline{\lambda_{max}}$ to equal μ appearing in (5); this argument is not exactly correct, however, since μ is defined from $\overline{C_N}$ where rare clusters with very large C_N can dominate. Our preliminary estimate of λ_{max} is 3.495 ± 0.002 where 662 clusters of size 10 000 were averaged and the error represents the standard error of the mean. While this number is not far from the estimate of μ, it is nonetheless significantly smaller; we believe this can be attributed to the dominance of rare clusters in μ just discussed.

If only λ_{max} matters, then it is easy to see that the exponent γ has to be 1. If we expand the S-component vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ appearing in (7) in terms of an orthonormal set of eigenvectors is not difficult to see that the leading term in the susceptibility

$$\chi(K) = \sum_{N=0}^{\infty} \overline{C_N} K^N \tag{10}$$

can be extracted in the limit $K \to 1/\mu^- = 1/\overline{\lambda_{max}}$ giving the asymptotic behaviour:

$$\chi(K) \sim (1 - \mu K)^{-1}. \tag{11}$$

In conclusion we have numerically investigated the mean end-to-end distance and number of chains for the ideal chain problem on the percolation cluster at the critical threshold p_c in two dimensions. We have showed that this problem does not belong to the same universality class as the corresponding random walk problem. We believe that this difference, besides its intrinsic interest as a theoretical model, could be also of real physical interest in systems like polymers in solution in a situation where the excluded volume effect is weak.

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