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Fractals Meet Fractals: Self-Avoiding Random Walks on Percolation Clusters

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The scaling behavior of linear polymers in disordered media, modelled by self-avoiding walks (SAWs) on the backbone of percolation clusters in two, three and four dimensions is studied by numerical simulations. We apply the pruned-enriched Rosenbluth chain-growth method (PERM). Our numerical results yield estimates of critical exponents, governing the scaling laws of disorder averages of the configurational properties of SAWs, and clearly indicate a multifractal spectrum which emerges when two fractals meet each other.

1. INTRODUCTION

Self-avoiding walks (SAWs) on regular lattices provide a successful description of the universal configurational properties of polymer chains in good solvent [1,2]. In particular, the average square end-to-end distance $\langle R^2 \rangle$ of SAWs with N steps obeys the scaling law

$$\langle R^2 \rangle \sim N^{2\nu_{\mathrm{SAW}}}, \tag{1}$$

where the universal exponent $\nu_{\mathrm{SAW}} > 1/2$ only depends on the space dimension d. For regular lattices, its value is well established ($\nu_{\mathrm{SAW}} = 3/4, 0.5882(11), 1/2$ for $d = 2, 3, \geq 4$). New challenges have been raised recently in studies of biopolymers in natural cellular environments, which are usually very crowded by many other biochemical species occupying a large fraction of the total volume [3]. In a minimalistic description, we assume here this "volume exclusion" to be random and frozen, i.e., quenched, and model the available space for the SAWs by site percolation clusters on hypercubic lattices at the percolation threshold $p_c = 0.592\,746, 0.311\,60, 0.196\,88$ in $d = 2, 3, 4$. Note that a percolation cluster itself is a fractal object with fractal dimension $d^B_{p_c}$ dependent on the space dimension d. The scaling law (1) still holds, but with an exponent $\nu_{p_c} \neq \nu_{\mathrm{SAW}}$ [4–16].

When studying physical processes on complicated fractal objects, one often encounters the situation of coexistence of a family of singularities, each associated with a set of different fractal dimensions [17]. In these problems, an infinite set of critical exponents is needed to characterize the different moments of the distribution of observables, which scale independently. These peculiarities are usually referred to as multifractality [18]. Multifractal properties arise in many different contexts, for example in studies of

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turbulence in chaotic dynamical systems and strange attractors [18,19], human heartbeat dynamics [20], Anderson localization transition [21], etc.

Although the behavior of SAWs on percolative lattices served as a subject of numerous numerical and analytical studies since the early 80th, not enough attention has been paid to clarifying the multifractality of the problem. It was only recently proven in field-theoretical studies [12,13] that the exponent ν_{p_c} alone is not sufficient to completely describe the peculiarities of SAWs on percolation clusters. Instead, a whole spectrum $\nu^{(q)}$ of multifractal exponents emerges [13]:

$$\nu^{(q)}=\frac{1}{2}+\left(\frac{5}{2}-\frac{3}{2^q}\right)\frac{\varepsilon}{42}+\left(\frac{589}{21}-\frac{397}{14\cdot 2^q}+\frac{9}{4^q}\right)\left(\frac{\varepsilon}{42}\right)^2, \tag{2}$$

with $\varepsilon = 6 - d$. Note that putting $q = 0$ in (2), we restore an estimate for the dimension $d^B_{p_c}$ of the underlying backbone of percolation clusters via $\nu^{(0)} = 1/d^B_{p_c}$, and $\nu^{(1)}$ gives us the exponent ν_{p_c}, governing the scaling law for the averaged end-to-end distance of SAWs on the backbone of percolation clusters. In the present paper, we report a careful computer simulation study of SAWs on percolation clusters.

2. METHODS

We consider site percolation on regular lattices of edge lengths up to $L_{\max}$=400, 200, 50 in dimensions d=2, 3, 4, respectively. Each site of the lattice is occupied randomly with probability p_c and empty otherwise. To extract the backbone of a percolation cluster, we apply the algorithm proposed in Ref. [22].

We construct a SAW on percolation clusters, applying the pruned-enriched chain-growth algorithm [23–25]. We let a trajectory of SAW grow step by step, until it reaches some prescribed distance (say R) from the starting point. Then, the algorithm is stopped, and a new SAW grows from the same starting point. In such a way, we are interested in constructing different possible trajectories with fixed end-to-end distance. For each lattice size L, we change R up to $\approx L/3$ to avoid finite-size effects, since close to lattice borders the structure of the backbone of percolation clusters is distorted and thus can falsify the SAW statistics.

Let us denote by $K(R)$ the total number of constructed SAW trajectories between 0 and R (we perform $\sim 10^6$ SAWs for each value of R). Then, for each site i of the backbone we sum up the portion of trajectories, passing through this site. In such a way, we prescribe a weight $w(i) = K(i)/K(R)$ to each site $i \in R$ of the underlying fractal cluster.

The multifractal moments $M^{(q)}$ are defined as follows:

$$M^{(q)} = \sum_{i\in R} w(i)^q. \tag{3}$$

Averaged over different configurations of the constructed backbones of percolation clusters, they scale as:

$$\overline{M^{(q)}} \sim R^{1/\nu^{(q)}}, \tag{4}$$

with exponents $\nu^{(q)}$ that do not depend on q in a linear or affine fashion, implying that SAWs on percolation clusters are multifractals. To estimate the numerical values of $\nu^{(q)}$ on the basis of data obtained by us, linear least-square fits are used.

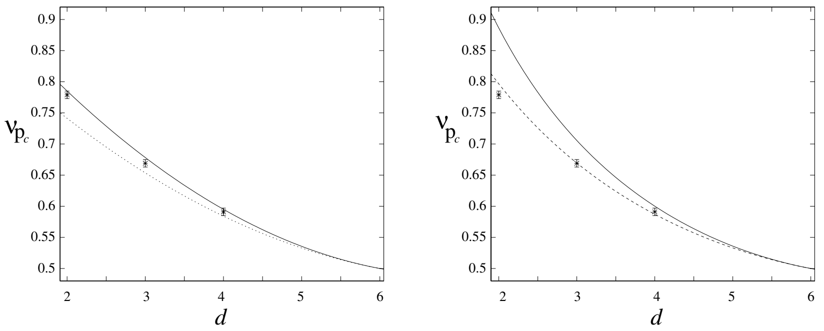

Figure 1. Critical exponent ν_{p_c} of SAWs on percolation clusters as function of space dimension d; stars: numerical data, obtained by us. Left: Dotted line: analytical results of Janssen and Stenull (Eq. (2)), solid line: analytical results of Ref. [12]. Right: [1]/[2] Padé approximants of the same analytical results.

3. RESULTS

At $q = 0$ we just count the number of sites of the cluster of linear size R, and thus $1/\nu^{(0)}$ corresponds to the fractal dimension of the backbone $d^B_{p_c}$. Our results give $d^B_{p_c}(d{=}2) = 1.647 \pm 0.006$, $d^B_{p_c}(d{=}3) = 1.865 \pm 0.006$, $d^B_{p_c}(d{=}4) = 1.946 \pm 0.006$. At $q = 1$, we restore the value of the exponent ν_{p_c}, governing the scaling law of the end-to-end distance for SAWs on the backbone of percolation clusters. We obtain $\nu^{(1)}(d{=}2) = 0.779 \pm 0.006$, $\nu^{(1)}(d{=}3) = 0.669 \pm 0.006$, $\nu^{(1)}(d{=}4) = 0.591 \pm 0.006$, in perfect agreement with our recent numerical estimates [12,14–16] based on the scaling of the end-to-end distance with the number of SAW steps. Comparison of our results for ν_{p_c} to that of the analytical studies [12,13] are presented in Fig. 1.

The precision of our estimates decreases with increasing q. This problem turns out to be also especially crucial when exploring the moments with negative powers q: the sites with small probabilities to be visited, which are determinant in negative moments, are very difficult to probe.

Our estimates of the exponents $\nu^{(q)}$ for different q are presented in Fig. 2. These values appear to be in perfect correspondence with analytical estimates down to $d = 2$ dimensions, derived by applying Padé approximation to the $\varepsilon = 6 - d$-expansion (2), presenting the given series as ratio $[m]/[n]$ of two polynomials of degree m and n in ε. We used the [1]/[2] approximant, because it appears to be most reliable in restoring the known estimates in the limiting case $q = 0$. A direct use of the expression (2) gives worse results, especially for low dimensions d where the expansion parameter $\varepsilon = 6 - d$ is large.

4. CONCLUSIONS

To conclude, we have shown numerically that SAWs residing on the backbone of percolation clusters give rise to a whole spectrum of singularities, thus revealing multifractal

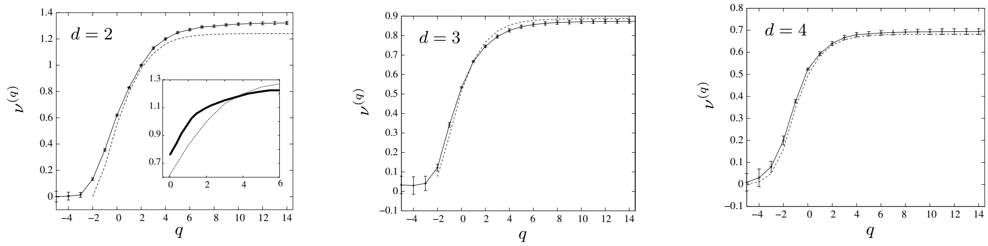

Figure 2. Spectrum of multifractal exponents $\nu^{(q)}$ as function of q in $d = 2, 3, 4$. The dotted lines present [1]/[2] Padé approximants to the analytical results of Janssen and Stenull (Eq. (2)). The inset for $d = 2$ shows a comparison with results from Ref. [26] (bold solid line).

properties. To completely describe peculiarities of the model, the multifractal scaling should be taken into account. We have found estimates for the exponents, governing different moments of the weight distribution, which scale independently.

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