# Structure of self–avoiding walks on percolation clusters at criticality

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## Abstract

The structure of linear polymers modelled by self–avoiding random walks (SAW) on the backbone of two–dimensional percolation clusters at criticality is studied. To this end, all possible SAW configurations of $N$ steps on a single backbone configuration are enumerated exactly, and averages over many backbone configurations are performed to extract the mean quantities of interest. We determine the critical exponents describing the structure of SAW, both in Euclidean and topological space, and the corresponding mean distribution functions for the end–to–end distance after $N$ steps. A relation between the exponents characterizing the asymptotic shape of these distributions and those describing the total number of SAW of $N$ steps on the backbone is suggested and supported by numerical results.

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## I. INTRODUCTION

Linear polymers embedded in disordered media constitute one of the most challenging problems in the physics of polymers. Indeed, this subject is relatively young as compared to the more traditional and extensively studied one of linear polymers, modelled by self–avoiding random walks (SAW), embedded in a regular system where no 'external' constraints are imposed on the chains (Flory 1949, Fisher 1966, de Gennes 1979, Doi and Edwards 1986, des Cloizeaux and Jannink 1990).

The study of linear polymers in a random medium is of practical interest for understanding the transport properties of polymeric chains in porous media, such as in enhanced oil recovery, gel electrophoresis, gel permeation chromatography, etc. (Doi and Edwards 1986, Dullien 1979, Andrews 1986, Baumgärtner 1995). In this respect, it is useful to learn about the static or conformational properties of linear chains in the presence of quenched disorder, i.e. how the surrounding structural disorder influences their asymptotic shape. As a quite general model of a random medium, percolation (Flory 1941, Stauffer and Aharony 1992, Sahimi 1994, Bunde and Havlin 1996) represents the simplest and mostly used one.

The question of interest is whether the statistical behavior of SAW change in the presence of structural disorder (modelled by lattice percolation clusters), with respect to their known behavior on regular lattices. There is a quite general concensus that it is only at the percolation threshold that non–trivial changes can be expected. In other words, the 'critical' exponents (to be defined below) describing the shape of SAW at the percolation threshold are different than in the case of a regular lattice (Nakanishi 1994, Barat and Chakrabarti 1995).

In this work, we consider SAW on percolation clusters at criticality in two dimensions. Since we aim at describing 'infinitely' long chains, we study them directly on the backbone of the clusters, where dangling ends are absent on all length scales. More precisely, we enumerate all possible SAW configurations of $N$ steps for a single backbone, and then avegrage over many different backbone configurations to extract the mean quantities of

interest. We determine the critical exponents describing the structure of SAW and the corresponding mean distribution function for the end–to–end distance after $N$ steps.

The paper is organized as follows. In Section II, we briefly review the main relevant properties of SAW on regular lattices. In Section III, we describe the percolation model employed and the corresponding backbone. In Section IV, we consider SAW on the backbone of percolation clusters at criticality. The structural functions and the total number of SAW configurations are obtained. Finally, in Section V we conclude with a brief summary of our main results.

## II. SAW ON REGULAR LATTICES

As a simple model for linear polymers in a good solvent we consider self–avoiding random walks (SAW) on regular lattices in $d$ dimensions. The structure and statistical properties of SAW have been studied extensively in the past decades (for general reviews see e.g. de Gennes 1979, des Cloizeaux and Jannink 1990). In what follows, we briefly review the main known results relevant for our present study.

Consider SAW of $N$ steps on a lattice. A quantity which characterizes the spatial extension of the chain can be obtained by calculating the end–to–end distance $r(N)$. By averaging $r(N)$ over all possible $N$–steps walks one obtains

$$\bar{r}(N) \sim N^{\nu} \tag{1}$$

where $\nu$ is a universal exponent (independent of the lattice type and depends only on $d$) and is given by $\nu \cong 3/(d+2)$, for $1 \leq d \leq 4$, as suggested by Flory (1949). Actually, the Flory formula yields the exact result in one and two dimensions, and predicts the correct value for the critical dimension, $d = 4$. Indeed, for $d \geq 4$, SAW become equivalent to simple random walks (RW) and $\nu = 1/2$. In three dimensions, it agrees quite well with the best numerical estimate, $\nu = 0.592 \pm 0.004$ (Guttmann 1989).

Linear chains generated by SAW, which we refer to as SAW–chains, are random linear fractals having a fractal dimension $d_f = 1/\nu$ (Havlin and D. Ben–Avraham 1987). For $d \geq 4$,

the fractal dimension $d_f$ sticks at the value $d_f = 2$ as for chains generated by simple random walks, referred to as RW–chains.

A more detailed information about the spatial structure of SAW is given by the probability $P(r, N)$ that after $N$ steps the end–to–end distance of a SAW is equal to $r$. This quantity obeys the scaling form (de Gennes 1979, des Cloizeaux and Jannink 1990)

$$P(r, N) = \frac{1}{r}\ f(r/N^{\nu}) \tag{2}$$

and is normalized according to $\int \mathrm{d}r\ P(r, N) = 1$. The analytic form of the scaling function $f(x)$ is known asymptotically

$$f(x) \sim x^{g_1+d}, \qquad x \ll 1 \tag{3}$$

where $g_1 = (\gamma - 1)/\nu$ (des Cloizeaux 1974), $\gamma$ is the second universal exponent for SAW (see below) and

$$f(x) \sim x^{g_2+d}\ \exp(-c\ x^{\delta}), \qquad x \gg 1 \tag{4}$$

where $g_2 = \delta\ [d(\nu - 1/2) - (\gamma - 1)]$ (McKennzie and Moore 1971) and $\delta = 1/(1 - \nu)$ (Fisher 1966).

The critical exponent $\gamma$ ($\geq 1$) is related to the total number $C_N$ of SAW configurations of $N$ steps by

$$C_N \sim A\ \mu^N\ N^{\gamma-1} \tag{5}$$

where $\mu$ is the effective coordination number of the lattice and is not universal, and $A$ is a constant. Numerical results yield $\mu = 2.6385 \pm 0.0001$ for the square lattice (Guttmann and Wang 1991, Masand, Wilensky, Massar, and Redner 1992). The fact that $\mu < 3$ means that the self–avoiding condition imposes further constraints to the walks in addition to the obvious one that the walk can not make a step to the direction where it just comes from. The latter would yield $\bar{\mu} = 2d - 1$ for hypercubic lattices.

The self–avoiding condition thus reduces dramatically the value of $C_N$ as compared to the case of simple walks for which $\mu = 2d$ on hypercubic lattices, yielding simultaneously a small

enhancement factor $N^{\gamma-1}$. For dimensions $d \geq 4$, however, $\gamma = 1$ since the excluded-volume restriction becomes irrelevant above the critical dimension.

The exponent $\gamma$ is known exactly for $d = 2$, $\gamma = 43/32$ (Niehnhuis 1982). A good approximation for $\gamma$ has been suggested recently, $\gamma = 1 + (4-d)/6$, for $1 < d \leq 4$, and $\gamma = 1$ for $d \geq 4$ (Roman 1995). This expression agrees remarkably well with the suggested exact value in $d = 2$, and with the best numerical estimates presently available, i.e. $\gamma = 1.33 \pm 0.02$ in $d = 2$ (Woo and Lee 1991), and $\gamma = 1.161 \pm 0.001$ in $d = 3$ (Guttmann 1989).

As we will see below, it is useful to study the behavior of the quantity $(\ln C_N)/N$ when considering polymers embedded in a disordered medium. It is therefore instructive to study the same quantity in the case of a regular lattice. We consider here the square lattice for which exact enumeration results for $C_N$ are available so far for $N \leq 34$ (Guttmann and Wang 1991, Masand et al. 1992). Using these values, we have plotted $(\ln C_N)/N$ versus $N$ as shown in Fig. 1. The continuous line corresponds to a numerical fit obtained in the range $10 \leq N \leq 34$ with the expression

$$\frac{1}{N} \ln C_N = \frac{\ln A}{N} + \ln \mu + \frac{\gamma - 1}{N} \ln N \tag{6}$$

yielding $\mu = 2.641 \pm 0.010$, $\gamma = 1.30 \pm 0.05$ and $A = 1.35 \pm 0.05$. Thus, compared to the asymptotic values $\mu = 2.6385 \pm 0.0001$ and $\gamma = 43/32$, our fit values differ by less than 0.09% from $\mu$ and by about 3% from $\gamma$, respectively.

We proceed by describing the underlying random structure in which SAW will be embedded.

## III. THE BACKBONE OF A PERCOLATION CLUSTER

Consider now the case in which the linear polymers are embedded in a random medium. In our simplified lattice model, this corresponds to having randomly sites which are blocked, i.e. are not available to the SAW. The natural model in this case is percolation (Flory 1941, Stauffer and Aharony 1992, Sahimi 1994, Bunde and Havlin 1996).

In our calculations we consider a square lattice of unit lattice constant, and generate large percolation clusters using the Leath growth method (Leath 1976, Alexandrowics 1980). The growth starts at the seed (origin of coordinates), whose nearest–neighbor sites can be either occupied with probability $p$ (they become cluster sites), or blocked (they can not be occupied later) with probability $1-p$. Thus, in the first grow step sites which are at distance $r=1$ from the seed can be occupied. It is customary to refer to them as belonging to the first grow 'shell'. In the second step, the growth starts again from each of the sites at the first shell. Then, sites which are at distance $r=2$ or $r=\sqrt{2}$ can be occupied. The new cluster sites generated in this second growth step belong to the second shell. We say that they are at the 'chemical' distance $\ell=2$ from the seed. Repeating this process again and again from the last shell of cluster sites, one can generate large percolation clusters up to the maximum number of shells required. Note that the cluster sites belonging to a given shell are at the same chemical distance $\ell$ from the seed, while their corresponding Euclidean distances $r$ from the seed can be very different from each other.

Since we aim at describing infinitely long SAW–chains on a percolation cluster, we can disregard the singly connected substructures, i.e., dangling ends, from the cluster where long SAW–chains can get stuck. Thus, we are confronted with the determination of the backbone of the cluster. Once a percolation cluster having the required maximum number of shells has been generated, we take one of the sites at the last grown shell at random, say site $A$, and determine the backbone of the cluster between $A$ and the seed (Herrmann, Hong, and Stanley 1984, Porto, Bunde, Havlin, and Roman 1997) (Fig. 2a).

Before proceeding with our discussion on SAW, we review some of the basic structural properties of the backbone at the critical concentration $p_{\rm c}$. Fig. 2b illustrates the two possible metrics which can be defined on the backbone for an arbitrary backbone site $B$, i.e. its Euclidean distance $r$ and its chemical distance $\ell$ from the seed. On average, the mean chemical distance of backbone sites at distance $r$ from the seed scales as (Pike and Stanley 1981, Havlin and Ben–Avraham 1987)

$$\langle \ell \rangle \sim r^{d_{\min}} \tag{7}$$

where $d_{\min} = 1.130 \pm 0.004$ in two dimensions (Herrmann and Stanley 1988, Neumann and Havlin 1988). Thus, Eq. (7) yields the scaling relation between the two metrics, which will be used in the following section. Finally, the backbone has a fractal dimension $d_\ell^{\rm B} = 1.45 \pm 0.01$ in $\ell$–space, yielding the value $d_f^{\rm B} = d_\ell^{\rm B} d_{\min} = 1.64 \pm 0.02$ in $r$–space (Porto et al. 1997).

## IV. SAW ON THE BACKBONE OF PERCOLATION

Now consider SAW on the backbone of a percolation cluster (Fig. 2c). For convenience, we study the case in which one end of the SAW is kept fixed at the seed. After $N$ steps, the SAW–chain reaches a backbone site located at Euclidean distance $r$ and chemical distance $\ell$ from the seed, yielding the end–to–end distances $r(N)$ and $\ell(N)$, respectively (see Fig. 2c).

### A. The critical exponents $\nu_r$ and $\nu_\ell$

By considering all SAW–chains of $N$ steps on the given backbone, we obtain the average quantities $\bar{r}(N)$ and $\bar{\ell}(N)$, respectively. A second average over different backbone configurations yields the final quantities,

$$\langle \bar{r}(N) \rangle \sim N^{\nu_r} \tag{8}$$

and

$$\langle \bar{\ell}(N) \rangle \sim N^{\nu_\ell} \tag{9}$$

where, according to Eq. (7), the critical exponents $\nu_r$ and $\nu_\ell$ are related to each other by

$$\nu_r = \frac{\nu_\ell}{d_{\min}}. \tag{10}$$

It is now generally accepted that at the percolation threshold $p_{\rm c}$, SAW belong to a different universality class than for regular lattices. It is found that in $d = 2$, the value of

$\nu_r$ is definitely larger than $\nu$ (Nakanishi 1994, Barat and Chakrabarti 1995). Some authors conclude that $\nu_r = 0.76 \pm 0.08$ (Meir and Harris 1989), $\nu_r = 0.77 \pm 0.02$ (Roman, Dräger, Bunde, Havlin, and Stauffer 1995), $\nu_r = 0.77 \pm 0.01$ (Woo and Lee 1991, Vanderzande and Komoda 1992) and $\nu_r = 0.775 \pm 0.005$ (Rintoul, Moon, and Nakanishi 1994), while others have proposed slightly larger values, i.e. $\nu_r = 0.78 \pm 0.01$ (Nakanishi and Moon 1992) and $\nu_r = 0.783 \pm 0.003$ (Grassberger 1993). Away from $p_c$, it is believed that the standard universality class is recovered, i.e. $\nu_r = \nu$ for $p > p_c$ (Nakanishi 1994, Barat and Chakrabarti 1995).

Our numerical results for $\langle \bar{r}(N) \rangle$ and $\langle \bar{\ell}(N) \rangle$ are reported in Fig. 3, from which we obtain

$$\nu_r = 0.78 \pm 0.02, \qquad \text{and} \qquad \nu_\ell = 0.89 \pm 0.01. \tag{11}$$

From the result for $\nu_\ell$ and the relation Eq. (10) we obtain a better estimate for $\nu_r$ as

$$\nu_r = \frac{\nu_\ell}{d_{\min}} = 0.786 \pm 0.010. \tag{12}$$

This result is in good agreement with the values reported by Nakanishi and Moon (1992), and Grassberger (1993). We proceed with the discussion of the end–to–end distribution functions both in $r$– and in $\ell$–space.

### B. The structural functions $P_B(r, N)$ and $P_B(\ell, N)$

For each backbone, we consider again all possible SAW–chains of $N$ steps and determine the probability $P_B(r, N)$ that the $N$th step reaches a backbone site at a distance $r$ from the seed. By performing a configurational average over many backbone configurations we obtain the quantity $\langle P_B(r, N) \rangle$, which is plotted in Fig. 4.

We find that $\langle P_B(r, N) \rangle$ is a scaling function of the variable $x = r/N^{\nu_r}$, i.e.

$$\langle P_B(r, N) \rangle = \frac{1}{r} \, f_B(x),$$

in agreement with a previous work (Roman et al. 1995). The numerical results suggest the following form for $f_B(x)$,

$$f_{\rm B}(x) \sim x^{g_1^r + d_f^{\rm B}}, \qquad x < 1 \tag{13}$$

and

$$f_{\rm B}(x) \sim x^{g_2^r + d_f^{\rm B}} \ \exp[-a\ x^{\delta_r}], \qquad x > 1. \tag{14}$$

We obtain, $g_1^r + d_f^{\rm B} = 2.2 \pm 0.2$, $g_2^r + d_f^{\rm B} = 3.1 \pm 0.4$, and $\delta_r = 4.9 \pm 0.3$, the latter is consistent with the value $\delta_r = 1/(1-\nu_r) = 4.7 \pm 0.2$. Using the value $d_f^{\rm B} = 1.64 \pm 0.02$ we find, $g_1^r = 0.56 \pm 0.20$ and $g_2^r = 1.46 \pm 0.40$.

More accurate are the results for the structural function in $\ell$–space, $\langle P_{\rm B}(\ell, N)\rangle$. These are shown in Fig. 5, suggesting the following scaling behavior as a function of $\ell/N^{\nu_\ell}$ (Roman et al. 1995)

$$\langle P_{\rm B}(\ell, N)\rangle \sim \frac{1}{\ell}\left(\frac{\ell}{N^{\nu_\ell}}\right)^{g_1^\ell + d_\ell^{\rm B}}, \qquad \ell/N^{\nu_\ell} < 1 \tag{15}$$

and

$$\langle P_{\rm B}(\ell, N)\rangle \sim \frac{1}{\ell}\left(\frac{\ell}{N^{\nu_\ell}}\right)^{g_2^\ell + d_\ell^{\rm B}} \exp[-b\ (\ell/N^{\nu_\ell})^{\delta_\ell}], \qquad \ell/N^{\nu_\ell} > 1 \tag{16}$$

and is normalized according to $\int {\rm d}\ell\ \langle P_{\rm B}(\ell, N)\rangle = 1$. We obtain $g_1^\ell + d_\ell^{\rm B} = 1.9 \pm 0.1$, $g_2^\ell + d_\ell^{\rm B} = 2.85 \pm 0.40$, and $\delta_\ell = 9.5 \pm 0.5$, the latter is consistent with the result $\delta_\ell = 1/(1-\nu_\ell) = 9.09 \pm 0.90$. Using the value $d_\ell^{\rm B} = 1.45 \pm 0.01$ we find, $g_1^\ell = 0.45 \pm 0.10$ and $g_2^\ell = 1.40 \pm 0.40$.

Actually, the values for $g_1^\ell$ and $g_1^r$ are related to each other by (Roman et al. 1995)

$$g_1^r = g_1^\ell\ d_{\rm min} \tag{17}$$

yielding the better estimate $g_1^r = 0.51 \pm 0.10$.

### C. The total number of configurations $C_{N,{\rm B}}$

In the following, we try to relate the exponent $g_1^r$ to other critical exponents describing SAW on the backbone, similarly as for regular systems (see Eq. (3)). This leads us to study the total number of SAW configurations on the backbone, $C_{N,{\rm B}}$.

Due to the disordered structure of the backbone, the number $C_{N,\mathrm{B}}$ can fluctuate strongly among different backbone configurations. A better behaved quantity is $\ln C_{N,\mathrm{B}}$, hence we consider first the 'quenched' average $\langle \ln C_{N,\mathrm{B}} \rangle$. Indeed, the values of $\ln C_{N,\mathrm{B}}$ are approximately normally distributed, as indicated in Fig. 6a. The width of the distribution, $\sigma_N$, grows as a power of $N$ as shown in Fig. 6b, as

$$\sigma_N \cong \sigma_0 \; N^{\chi} \tag{18}$$

with $\sigma_0 = 0.45 \pm 0.02$ and $\chi$ seems to tend to $\chi = 1/2$ for large $N$.

Our numerical results further indicate that the location of the maximum of the Gaussian, i.e. $\langle \ln C_{N,\mathrm{B}} \rangle$, can be well described by the analytic form

$$\frac{1}{N} \langle \ln C_{N,\mathrm{B}} \rangle = \frac{\ln B_0}{N} + \ln \mu_0 + \frac{\gamma_0 - 1}{N} \ln N \tag{19}$$

as shown in Fig. 7a. The fit yields the values $\mu_0 = 1.456 \pm 0.01$, $\gamma_0 = 1.26 \pm 0.05$ and $B_0 = 1.26 \pm 0.05$. Our value for $\mu_0$ agrees well with the result $\mu_{\mathrm{MC}} = 1.459 \pm 0.003$ obtained by generating SAW with Monte Carlo methods (Woo and Lee 1991). In the latter case, the most probable SAW configurations are actually generated, which correspond to our quenched average results. Our value for $\gamma_0$ is also consistent with $\gamma_{\mathrm{MC}} = 1.31 \pm 0.03$ (Woo and Lee 1991).

Let us consider next the annealed average, i.e. $\langle C_{N,\mathrm{B}} \rangle$. A good fit to the numerical results is obtained with the expression

$$\frac{1}{N} \ln \; [\langle C_{N,\mathrm{B}} \rangle] = \frac{\ln B_1}{N} + \ln \mu_1 + \frac{\gamma_1 - 1}{N} \ln N \tag{20}$$

yielding $\mu_1 = 1.565 \pm 0.01$, $\gamma_1 = 1.34 \pm 0.05$ and $B_1 = 1.24 \pm 0.05$, as shown in Fig. 7b. It is interesting to note that our value for $\mu_1$ is consistent with the suggested annealed result $\mu_{\mathrm{ann}} = p_c \; \mu$, where $p_c = 0.59274$ and $\mu = 2.6385$ (Harris 1983, Woo and Lee 1991, Grassberger 1993).

To characterize the fluctuations of $C_{N,\mathrm{B}}$ between different backbone configurations more generally, we study the moments $\langle C_{N,\mathrm{B}}^q \rangle^{1/q}$, where $q$ is a parameter. A similar study has

been performed for 'ideal' chains, i.e. chains which can intersect themselves, on percolation clusters at criticality. This model leads also to non–trivial results (Giacometti and Maritan 1994). It is easy to show that the quenched average can be obtained as

$$\langle \ln C_{N,\mathrm{B}} \rangle = \lim_{q \to 0} \ \ln \left[ \langle C_{N,\mathrm{B}}^q \rangle^{1/q} \right].$$

To proceed further, we make the ansatz

$$\langle C_{N,\mathrm{B}}^q \rangle^{1/q} \sim B_q \ \mu_q^N \ N^{\gamma_q - 1} \tag{21}$$

which is a generalization of Eq. (5), where $\mu_q$ are generalized effective coordination numbers of the backbone and $\gamma_q$ generalized enhancement exponents. In the following, we study Eq. (21) both analytically and numerically.

First, we evaluate the moments analytically assuming a log–normal distribution for $C_{N,\mathrm{B}}$. The result can be expected to be accurate only for $|q| \to 0$, since in this limit the moments are dominated by the maximum of the distribution, which is well described by a Gaussian shape. Within the Gaussian approximation we find,

$$\langle C_{N,\mathrm{B}}^q \rangle^{1/q} = \exp \langle \ln C_{N,\mathrm{B}} \rangle \ \exp \left( \frac{1}{2} q \sigma_0^2 N^{2\chi} \right), \qquad |q| \ll 1, \tag{22}$$

that has the form assumed in Eq. (21). Indeed, using Eq. (19), we obtain

$$\mu_q = \mu_0 \ \left( 1 + \frac{1}{2} q \sigma_0^2 \ N^{-(1-2\chi)} + O(q^2) \right) \tag{23}$$

which depends explicitely on $q$ and

$$\gamma_q = \gamma_0 \tag{24}$$

which does *not* depend on $q$. For $|q| \gg 1$, the moments will depend sensitively on the tails of the distribution which are not Gaussian in shape, and departures from the above results can be expected.

Next, we studied the moments $\langle C_{N,\mathrm{B}}^q \rangle^{1/q}$ for $|q| \leq 2$ numerically, and fitted them following our ansatz Eq. (21) according to the expression

$$\frac{1}{N}\ln\ \left[\langle C^q_{N,\mathrm{B}}\rangle^{1/q}\right] = \frac{\ln B_q}{N} + \ln\mu_q + \frac{\gamma_q - 1}{N}\ln N. \tag{25}$$

As one can see in Fig. 8a, the fits are quite satisfactory. Quantitatively, $\gamma_q$ tends to increase slightly as a function of $q$ for $q \geq -1$, displaying a more pronounced dependence for $q < -1$ where $\gamma_q \to 1$. The pre-factors $B_q$ turn out to be rather stable, varying in the range $1.24 < B_q < 1.26$ in a non–monotonous way. Regarding the fit values for $\mu_q$, they are consistent with the theoretical predictions expected for $|q| \to 0$ in the case $\chi = 1/2$, $\mu_q = \mu_0(1+q\sigma_0^2/2)$, as shown in Fig. 8b. For values $q \ll -1$, we found that $\mu_q \to 1$, corresponding to backbones which are almost linear in shape, while for $q \gg 1$, corresponding to more 'compact' backbones, $\mu_q$ remained well below its value $\mu$ for the square lattice.

According to these results we conclude that $C_{N,\mathrm{B}}$ is likely to display multifractal behavior. The multifractality is caused by the underlying multiplicative process characterized by an infinite hierarchy of effective coordination numbers $\mu_q$, which depend on $q$. Note that the term linear in $q$ in Eq. (23) would vanish for $N \to \infty$ if $\lim_{N\to\infty} 2\chi < 1$. In that case the log–normal approximation would yield standard behavior, i.e. absence of multifractal behavior asymptotically.

Finally, one can estimate values of the exponent $g_1^r$ by assuming a 'generalized' des Cloizeaux expression (cf. Eq. (3)) of the form

$$g_1^r \cong \frac{\gamma_1 - 1}{\nu_r}. \tag{26}$$

Using our value $\gamma_1 = 1.34 \pm 0.05$, we find $g_1^r = 0.43 \pm 0.05$, in good agreement with the numerical result Eq. (17).

## V. CONCLUSIONS

We have studied structural properties of SAW on the backbone of percolation clusters at criticality in two dimensions using an exact enumeration method. We find that the mean end–to–end distance in $\ell$–space, $\langle\bar{\ell}(N)\rangle \sim N^{\nu_\ell}$ with $\nu_\ell = 0.89 \pm 0.01$. From this result we

obtain the exponent $\nu_r = \nu_\ell / d_{\min} = 0.786 \pm 0.010$, describing the corresponding behavior in $r$–space, $\langle \bar{r}(N) \rangle \sim N^{\nu_r}$.

We have calculated the distribution function of the end–to–end distance in $r$–space, $\langle P_{\rm B}(r,N) \rangle$, and found to be described by a scaling function of the variable $x = r/N^{\nu_r}$, as

$$r \langle P_{\rm B}(r,N) \rangle \sim \begin{cases} x^{g_1^r + d_f^{\rm B}} & \text{for } x < 1, \\ x^{g_2^r + d_f^{\rm B}} \ \exp(-a \ x^{\delta_r}) & \text{for } x > 1. \end{cases}$$

Similarly, we have calculated the distribution $\langle P_{\rm B}(\ell,N) \rangle$ in $\ell$–space, obtaining the following scaling behavior as a function of $y = \ell / N^{\nu_\ell}$,

$$\ell \langle P_{\rm B}(\ell,N) \rangle \sim \begin{cases} y^{g_1^\ell + d_\ell^{\rm B}} & \text{for } y < 1, \\ y^{g_2^\ell + d_\ell^{\rm B}} \exp(-b \ y^{\delta_\ell}) & \text{for } y > 1, \end{cases}$$

The values of the corresponding critical exponents are reported in Table I.

Finally, we have studied the total number of SAW configurations of $N$ steps, $C_{N,{\rm B}}$. These numbers fluctuate strongly for different backbone configurations. We find that $\ln C_{N,{\rm B}}$ is approximately normally distributed having a width $\sigma_N \sim \sigma_0 \ N^{1/2}$, where $\sigma_0 = 0.45 \pm 0.02$. To characterize the fluctuations of $C_{N,{\rm B}}$ more generally, we have studied the moments $\langle C_{N,{\rm B}}^q \rangle^{1/q}$, where $q$ is a parameter. Our results suggest that

$$\langle C_{N,{\rm B}}^q \rangle^{1/q} \sim B_q \ \mu_q^N \ N^{\gamma_q - 1}$$

where $\mu_q$ are generalized effective coordination numbers of the backbone, $\gamma_q$ generalized enhancement exponents (cf. Eq. (5)) and $B_q$ pre–factors which depend weakly on $q$. Our results suggest that $1 \leq \mu_q \leq \mu$. However, the question whether $1 \leq \gamma_q \leq \gamma$ remains open. Within a log–normal approximation for $C_{N,{\rm B}}$ we find, for $|q| \to 0$, that $\mu_q = \mu_0 (1 + q \sigma_0^2 / 2)$, consistent with our numerical results. In addition, the present results suggest that on the backbone,

$$g_1^r \cong \frac{\gamma_1 - 1}{\nu_r}$$

generalizing the des Cloizeaux expression $g_1 = (\gamma - 1)/\nu$ valid on regular lattices (cf. Eq. (3)).

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## FIGURES

FIG. 1. The total number of SAW configurations of $N$ steps on the square lattice $C_N$ plotted as $(\ln C_N)/N$ versus $N$. The points correspond to the values of $C_N$ reported by Guttmann and Wang (1991), and Masand et al. (1992). The continuous line is a fit with the expression $(\ln C_N)/N = \ln A/N + \ln \mu + [(\gamma - 1)/N] \ln N$, yielding $\mu = 2.641 \pm 0.010$, $\gamma = 1.30 \pm 0.05$ and $A = 1.35 \pm 0.05$.

FIG. 2. SAW on percolation clusters at criticality. (a) A percolation cluster on the square lattice (light–grey squares) at the critical concentration $p_c \cong 0.59274$ and its corresponding backbone (dark–grey squares) between the seed $S$ (open circle) and a site $A$ at the last grown shell (full circle). (b) The Euclidean and the chemical metrics on the backbone shown in (a). An arbitrary backbone site $B$ (full circle) can be characterized either by its Euclidean distance $r$ or by its chemical distance $\ell$ from the seed $S$. In this case, $r = \sqrt{50}$ and $\ell = 12$. The line in white indicates the minimal path from $S$ to B. (c) An SAW of $N = 20$ steps (21 monomers) on the backbone shown in (b). One end of the SAW is taken to be fixed at the seed $S$ and the other is taken at site $B$. The black line connecting the full circles (monomers) indicate the linear polymer. This figure illustrates the way in which the quantities $r(N)$ and $\ell(N)$ can be determined on the backbone. In this example, $r(20) = \sqrt{50}$ and $\ell(20) = 12$.

FIG. 3. The mean end–to–end distance of SAW–chains on the backbone of percolation clusters at criticality in two dimensions. (a) $\langle \bar{r}(N) \rangle$ vs $N$, (b) $\langle \bar{\ell}(N) \rangle$ vs $N$ and (c) the successive slopes $\nu_\ell$ (full circles) and $\nu_r$ (full squares) vs $1/N$. Extrapolations of the points for $1/N \to 0$ yield our estimates $\nu_r = 0.78 \pm 0.02$ and $\nu_\ell = 0.89 \pm 0.01$. The straight lines in (a) and (b) are drawn as a guide and have the slopes $\nu_r = \nu_\ell / d_{\min} = 0.786$ and $\nu_\ell = 0.89$, respectively. Averages over $5 \cdot 10^4$ cluster configurations were performed. For each cluster, all SAW–chains were obtained for $N \leq 30$.

FIG. 4. The structural function $r\langle P_{\rm B}(r,N)\rangle$ versus the scaling variable $r/N^{\nu_r}$, with $\nu_r = 0.786$, for $N = 39$ (full diamonds) and $N = 40$ (full circles). Averages over $5\cdot 10^4$ backbone configurations were performed. The line in the range $r/N^{\nu_r} < 1$ has a slope $g_1^r + d_f^{\rm B} = 2.2 \pm 0.2$, and the one for $r/N^{\nu_r} > 1$ is a fit with Eq. (14), yielding $g_2^r + d_f^{\rm B} = 3.1 \pm 0.4$, $\delta_r = 4.9 \pm 0.3$ and $a = 0.79 \pm 0.02$.

FIG. 5. The structural function $\ell\langle P_{\rm B}(\ell,N)\rangle$ versus the scaling variable $\ell/N^{\nu_\ell}$, with $\nu_\ell = 0.89$, for $N = 39$ (full diamonds) and $N = 40$ (full circles). Averages over $5\cdot 10^4$ backbone configurations were performed. The line in the range $\ell/N^{\nu_\ell} < 1$ has a slope $g_1^\ell + d_\ell^{\rm B} = 1.9 \pm 0.1$, and the one for $\ell/N^{\nu_\ell} > 1$ is a fit with Eq. (16), yielding $g_2^\ell + d_\ell^{\rm B} = 2.85 \pm 0.40$, $\delta_\ell = 9.5 \pm 0.5$ and $b = 0.09 \pm 0.02$.

FIG. 6. Total number of SAW configurations, $C_{N,{\rm B}}$, on the backbone of percolation clusters in $d = 2$ at criticality. (a) The distribution of $\ln C_{N,{\rm B}}$ for $N = 10$ and 40. The lines are fits with the form $P(z) = (2\pi\sigma_N^2)^{-1/2}\ \exp[-(z-\bar z)^2/(2\sigma_N^2)]$, where $z = \ln C_{N,{\rm B}}$ and $\bar z = \langle \ln C_{N,{\rm B}}\rangle$. (b) The standard deviation $\sigma_N$ versus $N$. The straight line is a fit with the form $\sigma_N = \sigma_0\ N^{1/2}$, yielding $\sigma_0 = 0.45 \pm 0.02$. Here, averages over $10^5$ backbone configurations were performed.

FIG. 7. (a) The quenched average $\langle \ln C_{N,{\rm B}}\rangle$, plotted as $(1/N)\langle \ln C_{N,{\rm B}}\rangle$ versus $N$. The continuous line is the best fit with Eq. (19) yielding $\mu_0 = 1.456\pm0.010$, $\gamma_0 = 1.26\pm0.05$ and $B_0 = 1.26\pm0.05$. (b) The annealed average $\langle C_{N,{\rm B}}\rangle$, plotted as $(1/N)\langle C_{N,{\rm B}}\rangle$ versus $N$. The continuous line is the best fit with Eq. (20) yielding $\mu_1 = 1.565 \pm 0.010$, $\gamma_1 = 1.34 \pm 0.05$ and $B_1 = 1.24 \pm 0.05$.

FIG. 8. Generalized moments $\langle C_{N,{\rm B}}^q\rangle^{1/q}$ for SAW on the backbone of percolation clusters in $d = 2$ at criticality. (a) The quantity $(1/N)\ln\left[\langle C_{N,{\rm B}}^q\rangle^{1/q}\right]$ is plotted versus $N$, for $q$=2 (top), 1, 0.5, 0, -0.5, -1 and -2 (bottom). The lines are fits with Eq. (25). Some representative values for $\gamma_q$, in addition to those reported in Fig. 7, are: $\gamma_{-2} = 1.15$, $\gamma_{-1} = 1.25$ and $\gamma_2 = 1.36$. Values of $B_q$ are found to fluctuate in the range 1.24-1.26. (b) The effective coordination numbers $\mu_q$ versus $q$ obtained in (a). The straight line is the theoretical result $\mu_q = \mu_0(1 + q\sigma_0^2/2)$, expected for $|q| \to 0$ in the case $\chi = 1/2$, with $\mu_0 = 1.456$ and $\sigma_0 = 0.45$.

## TABLES

| $\nu_\ell$ | $\nu_r$ | $g_1^\ell$ | $g_1^r$ | $g_2^\ell$ | $g_2^r$ |
|---|---|---|---|---|---|
| $0.89 \pm 0.01$ | $0.786 \pm 0.010$ | $0.45 \pm 0.10$ | $0.51 \pm 0.10$ | $1.40 \pm 0.40$ | $1.46 \pm 0.40$ |

TABLE I. Values of the critical exponents for SAW on the backbone of percolation clusters at criticality in two dimensions. The values for $\nu_r$ and $g_1^r$ have been obtained from the relations $\nu_r = \nu_\ell / d_{\min}$ and $g_1^r = g_1^\ell \; d_{\min}$, where $d_{\min} = 1.130 \pm 0.004$ (Herrmann and Stanley 1988, Neumann and Havlin 1988). The numerical values for the exponents $\delta_\ell$ and $\delta_r$ are consistent, within the present accuracy, with the expressions $\delta_\ell = 1/(1-\nu_\ell)$ and $\delta_r = 1/(1-\nu_r)$, respectively.