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''Generalized des Cloizeaux'' exponent for self-avoiding walks on the incipient percolation cluster

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We study the asymptotic shape of self-avoiding random walks (SAW) on the backbone of the incipient percolation cluster in *d*-dimensional lattices analytically. It is generally accepted that the configurational averaged probability distribution function $\langle P_B(r,N)\rangle$ for the end-to-end distance r of an N step SAW behaves as a power law for $r\to 0$. In this work, we determine the corresponding exponent using scaling arguments, and show that our suggested ''generalized des Cloizeaux'' expression for the exponent is in excellent agreement with exact enumeration results in two and three dimensions.

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Linear polymers have a broad spectrum of applications in such different fields as biology, chemistry, and physics, see, e.g., [1–3], and theoretical work has been extensively documented in the literature [4–6]. More recently, strong interest has been drawn to the effects that environmental disorder may have on the configurational properties of such linear structures [7–9]. As a paradigmatic model of linear polymers, self-avoiding random walks (SAW) have captured the attention of researchers for decades and are currently extensively studied [4–6]. Structural disorder is generally modeled by percolation [10,11], and interesting effects are expected at the percolation threshold [8]. Since asymptotically long SAW can only exist on the backbone of the cluster, in which all dangling ends have been eliminated, one may study SAW directly on the backbone. For relatively short chains, one may still expect that the statistical properties of SAW do not depend on whether they are studied on the backbone alone or on the corresponding percolation cluster. In what follows, we adopt this point of view and study SAW directly on the backbone of the cluster.

On percolation clusters, one can distinguish between two different metrics, the usual Pythagorian one, or r-space metric, and the topological one, or ℓ-space metric, which have been extensively discussed in the literature [11–13]. The corresponding length scales are related by $\ell \sim r^{d_{\min}}$, where $d_{\min}$ is the fractal dimension of the shortest path [11].

The scaling behavior of SAW is characterized by the mean end-to-end distance after N steps. On structurally disordered systems such as percolation clusters, two types of averages need to be performed. One first averages over all SAW configurations of N steps on a single backbone starting from the same origin as obtained, e.g., by exact enumeration techniques [14], followed by a configurational average over many backbones. In r space, the former average is denoted as $\overline{r^2}(N)$, and the second one by $\langle \overline{r^2}(N)\rangle \sim N^{2\nu_r}$, which defines the exponent ν_r. Correspondingly, in ℓ space one has $\langle \overline{\ell}(N)\rangle \sim N^{\nu_\ell}$, where $\nu_\ell = \nu_r\, d_{\min}$.

More generally, one is interested in the configurational averaged probability distribution function (PDF) for the end−to−end distance on the backbone. In r-space, it is denoted as $\langle P_B(r,N)\rangle$, and is expected to obey the scaling form

$$\langle P_B(r,N)\rangle = \frac{1}{N^{\nu_r d_f^B}} f_r(r/N^{\nu_r}) \quad \text{for} \quad N \gg 1, \tag{1}$$

which is normalized according to $\int_0^\infty \mathrm{d}r\, r^{d_f^B-1}\langle P_B(r,N)\rangle = 1$, where d_f^B is the fractal dimension of the backbone. The scaling function $f_r(x)$ behaves as $f_r(x)\sim x^{g_1^r}$, for $x \ll 1$, and in this limit Eq. (1) becomes

$$\langle P_B(r,N)\rangle \sim \frac{1}{N^{\nu_r d_f^B}} \left(\frac{r}{N^{\nu_r}}\right)^{g_1^r} \quad \text{for} \quad r \ll N^{\nu_r}, \tag{2}$$

where g_1^r is the scaling exponent to which we draw our attention here. In ℓ space, the PDF obeys $\langle P_B(\ell,N)\rangle = N^{-\nu_\ell d_\ell^B} f_\ell(\ell/N^{\nu_\ell})$ and is normalized according to $\int_0^\infty \mathrm{d}\ell\, \ell^{d_\ell^B-1}\langle P_B(\ell,N)\rangle = 1$, with d_ℓ^B being the fractal dimension of the backbone in ℓ space, $d_\ell^B = d_f^B/d_{\min}$. The corresponding exponent in the case $\ell \ll N^{\nu_\ell}$ is denoted by g_1^ℓ and is related to g_1^r by $g_1^\ell = g_1^r/d_{\min}$ (see, e.g., [15,16]). The interest in studying the PDF $\langle P_B(\ell,N)\rangle$ is because fluctuations are definitely smaller in ℓ space than in r space, and more accurate results for g_1^r can be derived by determining g_1^ℓ and afterwards using the relation $g_1^r = g_1^\ell d_{\min}$.

In the case of regular lattices ($g_1^\ell = g_1^r = g_1$), des Cloizeaux [17] showed that $g_1 = (\gamma-1)/\nu_F$, where $\nu_F \cong 3/(d+2)$ is the Flory exponent [18] and γ describes the total number C_N of SAW configurations of N steps,

$$C_N \cong \mu^N N^{\gamma-1} \quad \text{for} \quad N \gg 1, \tag{3}$$

where μ is the effective coordination number of the lattice (see, e.g., [6]). Numerical results for SAW on the backbone of percolation clusters at criticality in two dimensions seem to be roughly consistent with the form $g_1^r = (\gamma_1-1)/\nu_r$ [15], where γ_1 is the corresponding enhancement exponent on the backbone. More recent results in three dimensions [16]

TABLE I. Critical exponents and fractal dimensions for the incipient percolation cluster, for spatial dimensions $d=2$, 3, and $d \geqslant 6$, from (a) exact results Ref. [21], (b) Monte Carlo simulations Ref. [22], (c) exact results Ref. [23], (d) Refs. [10,11], (e) Monte Carlo simulations Ref. [24], (f) Monte Carlo simulations Ref. [25], (g) Monte Carlo simulations Ref. [13], (h) Monte Carlo simulations Ref. [12], and (i) the relation $d_{\ell}^{B}=d_f^B/d_{\min}$. Here, $d_f=d-\beta/\nu$ is the fractal dimension of percolation clusters.

	$d=2$	$d=3$	$d\geqslant 6$
β	5/36(a)	0.417 ± 0.003(b)	1(c)
ν	4/3(a)	0.875 ± 0.008(b)	1/2(c)
d_f	91/48(a)	2.524 ± 0.008(b)	4(d)
d_f^B	1.6432 ± 0.0008(e)	1.87 ± 0.03(f)	2(d)
$d_{\min}$	1.1306 ± 0.0003(g)	1.374 ± 0.004(h)	2(d)
d_{ℓ}^{B}	1.446 ± 0.001(i)	1.36 ± 0.02(f)	1(d)

clearly disprove this relation, so the question remains whether a generalization of the des Cloizeaux expression can still provide an accurate framework for estimating the exponent g_1^r analytically. The goal of the present paper is to provide such a generalization of the des Cloizeaux relation valid in all dimensions.

To this end, we follow de Gennes [4] and study the probability $\langle P_B(a,N)\rangle$ that the Nth step of the SAW is on a backbone site located at a lattice distance $a=1$ from its starting point at $r=0$. This probability can be written as

$$\langle P_B(a=1,N)\rangle \sim \frac{\langle C_{N,B}(a=1)\rangle}{\langle C_{N,B}\rangle}, \tag{4}$$

where $\langle C_{N,B}(a=1)\rangle$ represents the (configurational) average number of SAW that, after N steps, arrive at a distance $a=1$ from the origin, and $\langle C_{N,B}\rangle$ denotes the total number of SAW of N steps. The latter is the configurational average analog of Eq. (3), with μ and γ replaced by the exponents μ_1 and γ_1. The index 1 reminds us of the underlying multifractal behavior of these two exponents for percolation systems [16] (see also Ref. [19]). We assume the former to be

$$\langle C_{N,B}(a=1)\rangle = \mu_1^N \left(\frac{a}{R}\right)^{d_f^B} F_B, \tag{5}$$

where $R\equiv\langle \overline{r^2}(N)\rangle^{1/2}\sim N^{\nu_r}$, and the factor $F_B\sim R^{-\kappa}\leqslant 1$ represents the additional difficulty of the N step SAW to return close to its starting point due to topological constraints caused by the statistical nature of the embedding structure. For regular lattices, this factor reduces to unity since in those cases there is no distinction between cluster and lattice sites, and the exponent d_f^B is replaced by the spatial dimensionality d of the lattice [4]. For deterministic fractals such as Sierpinski gaskets, the factor F_B is also expected to be unity, since in those cases the fractal structure embedding the SAW is also unique [20].

The exponent κ can be determined by considering first the probability that an arbitrary site belongs to the infinite cluster, P_∞. Near the percolation threshold p_c, P_∞ behaves as a function of the concentration p ($\geqslant p_c$) of occupied sites as [10,11]

$$P_\infty \sim (p-p_c)^\beta \sim \xi^{-\beta/\nu}, \tag{6}$$

where the correlation length ξ, diverging as $\xi\sim|p-p_c|^{-\nu}$ near p_c, is a measure of the linear size of the finite clusters in the system (or similarly, the mean distance between two sites on the same finite cluster), and ν is the correlation length exponent. Equation (6) suggests that the probability $P_\infty(L)$, to find a site belonging to the incipient cluster within a distance L from a given cluster site (and consequently at least one path connecting these two sites), scales as $P_\infty(L)\sim L^{-\beta/\nu}$ for $L<\xi$ [11]. Identifying the length scale L with the mean size R of the SAW, $L\sim R$, we obtain $F_B\sim R^{-\beta/\nu}$, i.e., $\kappa=\beta/\nu$. Accepted values [10–13, 21–25] for the critical exponents reported so far are summarized in Table I.

Using Eqs. (4),(5), and the above result for F_B, we find

$$\langle P_B(a=1,N)\rangle \sim \frac{\mu_1^N (a/R)^{d_f^B} F_B}{\mu_1^N N^{\gamma_1-1}} \sim \frac{1}{N^{\nu_r d_f^B}} \left(\frac{1}{N^{\nu_r}}\right)^{(\gamma_1-1)/\nu_r+\beta/\nu}, \tag{7}$$

and comparison with Eq. (2) yields

$$g_1^r = \frac{\gamma_1-1}{\nu_r} + \frac{\beta}{\nu}, \tag{8}$$

which is denoted as the generalized des Cloizeaux relation.

Numerical calculations based on exact enumeration techniques in two and three dimensions (taken from Ref. [16]) are reported in Fig. 1 for $\langle P_B(\ell,N)\rangle$. The corresponding numerical values for g_1^{ℓ} and g_1^r are summarized in Table II. The suggested relation (8) is in excellent agreement with the numerical data. Additionally, it should be noted that Eq. (8) yields the correct value expected when $d\geqslant 6$, i.e., $g_1^r=2$.

TABLE II. Results for SAW on the backbone of critical percolation clusters (from Ref. [16]). Note that the value of g_1^{ℓ} slightly differs from the value given in Ref. [16], as we determined it more accurately here by plotting $(N^{\nu_e})d_l^3\langle P_B(\ell,N)\rangle$, as shown in Figs. 1(b) and 1(d). The last line displays the present theoretical results from the generalized des Cloizeaux relation $g_1^r=(\gamma_1-1)/\nu_r+\beta/\nu$, Eq. (8).

	$d=2$	$d=3$	$d\geqslant 6$
ν_r	0.787 ± 0.010	0.662 ± 0.006	1/2
γ_1	1.34 ± 0.05	1.29 ± 0.05	1
g_1^r	0.56 ± 0.10	0.90 ± 0.10	2
g_1^{ℓ}	0.49 ± 0.05	0.67 ± 0.05	1
$g_1^r=g_1^{\ell}d_{\min}$	0.55 ± 0.06	0.92 ± 0.08	2
g_1^r (present conjecture)	0.54 ± 0.07	0.916 ± 0.080	2

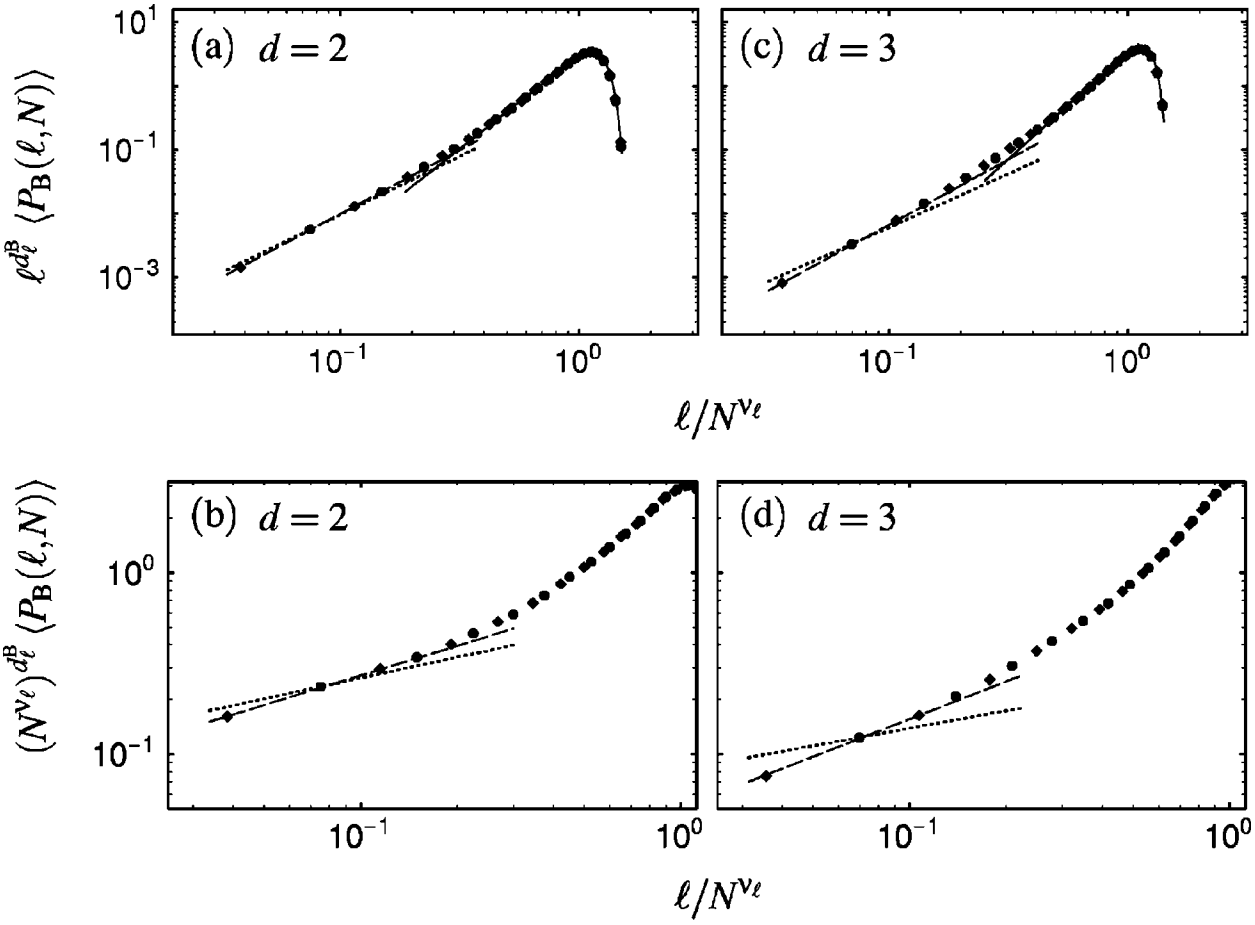

FIG. 1. Scaling plots of the PDF in ℓ space on the backbone of the incipient percolation cluster in (a),(b) $d=2$ and (c),(d) $d=3$, from the exact enumeration results of Ref. [16]. In (a) and (c), the whole PDF is shown, plotted as $\ell^{d_\ell^B}\langle P_B(\ell,N)\rangle$ versus ℓ/N^{ν_ℓ}, for $N=39$ (closed circles) and 40 (closed squares), averaged over 5×10^3 backbone configurations. In (b) and (d), the region with $\ell \ll N^{\nu_\ell}$ is shown in more detail, plotted as $\ell^{d_\ell^B}\langle P_B(\ell,N)\rangle/(\ell/N^{\nu_\ell})^{d_\ell^B}=(N^{\nu_\ell})^{d_\ell^B}\langle P_B(\ell,N)\rangle$ versus ℓ/N^{ν_ℓ} [26]. Case $d=2$: In (a) the solid line corresponds to the case $\ell \gg N^{\nu_\ell}$ and is not further discussed here (see [16] for details). For $\ell \ll N^{\nu_\ell}$ the dashed line in (b) has the slope 0.49 ± 0.05 and is a fit with the ansatz $(N^{\nu_\ell})^{d_\ell^B}\langle P_B(\ell,N)\rangle \sim (\ell/N^{\nu_\ell})^{g_1^\ell}$ for $\ell \ll N^{\nu_\ell}$ [cf. Eq. (2) and text], in very good agreement with the prediction $g_1^\ell=(\gamma_1-1)/\nu_\ell+\beta/(\nu d_{\min})\cong0.474$ [derived from Eq. (8) using the relation $g_1^\ell=g_1^r/d_{\min}$]. The dotted line is for illustration only and has the slope 0.382, resulting from the relation $(\gamma_1-1)/\nu_\ell\cong0.382$, in disagreement with the numerical results. Case $d=3$: Similarly to (b), in (d) the dashed line has the slope 0.67 ± 0.05, in excellent agreement with the prediction $g_1^\ell=(\gamma_1-1)/\nu_\ell+\beta/(\nu d_{\min})\cong0.666$. The dotted line has the slope 0.32, resulting from $(\gamma_1-1)/\nu_\ell\cong0.32$, clearly revealing the inadequacy of this relation to fit the numerical results.

Indeed, when $d\geqslant6$ the backbone of the incipient percolation cluster becomes topologically one-dimensional, since loops are irrelevant on large length scales, and one simply has $\gamma_1=1$. Thus, g_1^r is solely determined by the second term in Eq. (8). The value $g_1^r=2$ for $d\geqslant6$ can be understood by noting that in this case $F_B\sim(a/R)^{d_f^B}$ with $d_f^B=2$ for $d\geqslant6$, since SAW are equivalent to the embedding backbone and the probability to return close to the starting point just decreases as R^{-2}, i.e., $g_1^r=2$. The good agreement between Eq. (8) and the numerical results supports the ansatz made in Eq. (5).

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