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Self-avoiding walks on self-similar structures: finite versus infinite ramification

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Abstract

Self-avoiding walks (SAWs) generated by exact enumeration techniques are studied on the Sierpinski carpet ($d = 2$) and on the Sierpinski sponge ($d = 3$) (also called Sierpinski square lattices). A detailed comparison of the results for SAWs on these infinitely ramified fractals to SAWs on finitely ramified Sierpinski gaskets (Sierpinski triangular lattices), on regular lattices, and on the incipient percolation cluster is done, providing insight into the behaviour of SAWs on ordered and disordered structures. The SAWs on Sierpinski square lattices are found to display a kind of intermediate behaviour, sharing aspects of both SAWs on ordered and on fractal structures. As a consequence, a des Cloizeaux relation does *not* seem to hold for this structure, as opposed to its validity for SAWs on regular lattices, on Sierpinski triangular lattices and on the incipient percolation cluster.

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1. Introduction

Linear polymers made of similar monomer units in a diluted solution display only short-range (repulsive) interactions if the solvent is able to screen all long-range forces between them. In such a good solvent, the linear chain can be accurately modelled by a self-avoiding walk (SAW) (see [1–3] for a comprehensive review). SAWs are customarily studied on a lattice, for which many statistical properties are known so far (cf the above references). Some exponents characterizing the SAWs have even been established in exact form. For example, the Flory relation $\nu = 3/(d+2)$ [4] for the exponent ν, describing the scaling behaviour of the polymers' radius of gyration as a function of the number of monomers, has very recently been proved by Hueter [5] to be *exact* for SAWs in $d = 2$ and, furthermore, been rigorously generalized to $\nu = \max\{1/2, 1/4 + 1/d\}$ valid for any dimension $d \geqslant 2$ (correcting, for SAWs, the

approximate Flory result $\nu = 3/5$ in $d = 3$ to the exact value $\nu = 7/12$). Furthermore, many analytical relations between exponents are known [3], some of which are exact, others being conjectures or based on mean-field or scaling arguments. Together, these results provide a well-established framework to understand SAWs on regular lattices.

However, much less is known in the case of linear polymers embedded in disordered media. Typical examples of models studied so far include SAWs on the incipient percolation cluster [6–8], for which the exponents are known only numerically. These values are now established with quite high precision, and even some relations between them have been conjectured. For example, the so-called des Cloizeaux relation, first established for SAWs on regular lattices [9], has recently been generalized to SAWs on the incipient percolation cluster [10]. Despite these achievements, a full understanding of linear polymers in disordered media is still lacking.

For a better understanding of polymers in disordered media it is helpful to study SAWs on *deterministic* fractals. Here, results of renormalization group (RG) techniques are available, for example for Sierpinski gaskets [11, 12], hereafter denoted as Sierpinski triangular lattices for simplicity. However, these RG techniques are only applicable for *finitely* ramified structures such as the Sierpinski triangular lattices. For *infinitely* ramified structures, there is no RG result possible, and one has to rely on numerically evaluating SAWs on these fractals. Finite and infinite ramifications refer to the number of cut operations which are required to disconnect any given subset of the structure [13, 14]. For instance, for Sierpinski triangular lattices one needs to cut a finite number of bonds to do so, the upper limit of which is independent of the chosen subset.

The question therefore emerges of how do SAWs behave on such infinitely ramified fractals, and whether their behaviour differs from the case of finitely ramified structures. Good candidates to answer this quest are the so-called Sierpinski carpets (in $d = 2$) and Sierpinski sponges (in $d = 3$) [15–17]. For simplicity, these structures are summarized hereafter as Sierpinski square lattices.

There exist different versions of Sierpinski square lattices. These are usually distinguished by two integer numbers (n, k), where n is the length of the initiator and k refers to the number of subunits not present in the generator. Consequently, this means that $n^d - k$ subunits are present, so that the fractal dimension becomes

$$d_{\mathrm{f}}^{\mathrm{S}} = \frac{\ln(n^d - k)}{\ln n}. \tag{1}$$

Even after specifying (n, k), there is still the degree of freedom of *which* k out of n^d subunits are not present. This is quantified by the so-called lacunarity, which is a measure of the failure of a given fractal to be translationally invariant [14]. For our purposes, we choose the most common and symmetric (small lacunarity) configuration with $(n, k) = (3, 1)$ in $d = 2$ (the central subunit is not present) and $(n, k) = (3, 7)$ in $d = 3$ (the central subunit and its six nearest neighbour subunits are not present). An example of such a structure for $d = 2$ is given in figure 1. The critical exponents of SAWs are expected to depend both on the values of (n, k) and on the lacunarity, for example in more asymmetric (increased lacunarity) cases ν is known to be larger [15, 17].

In this paper we study SAWs on these Sierpinski square lattices in $d = 2$ and $d = 3$ using exact enumeration of all SAWs of length N. By doing this, we can draw conclusions regarding the role ramification plays on the statistical properties of SAWs. In particular, one of our aims is to elucidate whether a des Cloizeaux relation holds for infinitely ramified deterministic fractals. For completeness, we briefly review here previous results for SAWs on Sierpinski triangular lattices, as well as on regular lattices and on the incipient percolation

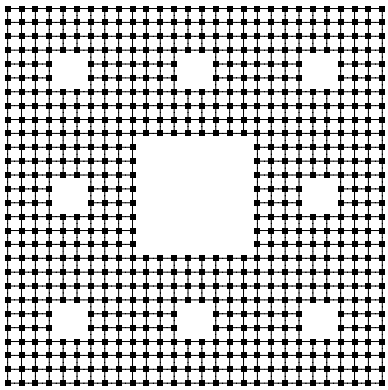

Figure 1. Illustration of the two-dimensional Sierpinski square lattice (also referred to as the Sierpinski carpet, corresponding to $(n, k) = (3, 1)$, see text) as obtained after the second iteration. The sites available to the SAW are shown as squares and the inter-connecting bonds are shown as lines.

cluster. Our calculations indicate that the behaviour of SAWs on Sierpinski square lattices is somehow intermediate between SAWs on regular lattices and on Sierpinski triangle lattices (see discussion in section 4).

The paper is organized as follows: in section 2 we discuss the expected scaling behaviours for the mean end-to-end chemical distance of the SAWs after N steps, the scaling forms of the probability distribution function (PDF) $P_{\mathrm{S}}(\ell, N)$, and the total number $C_{N,\mathrm{S}}$ of SAWs of length N. In section 3, we discuss the numerical procedure employed and report our exact enumeration results for the end-to-end distance (section 3.1), the PDF (section 3.2), and the total number of SAW configurations (section 3.3). Finally, in section 4, we summarize and discuss our main results and give our concluding remarks.

2. Theoretical results

To characterize the spatial extent of SAWs on a given structure, such as a Sierpinski square lattice, let us consider the topological end-to-end distance ℓ after N steps of the walk. Here we choose to study the topological or chemical distance ℓ over the Euclidean distance r due to its numerical convenience (note that for Sierpinski square lattices, ℓ and r are proportional to each other, $r \sim \ell$). By averaging over all possible walks starting at a given lattice point (using exact enumeration techniques) the mean end-to-end chemical distance $\overline{\ell}(N)$ is obtained. The latter is expected to scale as

$$\overline{\ell}(N) \sim N^{\nu_{\mathrm{S}}} \tag{2}$$

valid for $N \gg 1$, which defines the critical exponent ν_{S}. To obtain more detailed structural information of the SAWs, one can determine the probability $P_{\mathrm{S}}(\ell, N)\,\mathrm{d}\ell$ that a walk of length N has an end-to-end distance in the interval between ℓ and $\ell + \mathrm{d}\ell$. The corresponding PDF $P_{\mathrm{S}}(\ell, N)$ is expected to obey the scaling form

$$P_{\mathrm{S}}(\ell, N) \sim \frac{1}{\ell} F_{\mathrm{S}}\left(\frac{\ell}{\overline{\ell}(N)}\right) \tag{3}$$

where the scaling function $F_S(x)$ is expected to behave as

$$F_S(x) = \begin{cases} x^{g_1^S + d_f^S} & \text{for } x \ll 1 \\ x^{g_2^S + d_f^S} \exp[-c_S x^{\delta_S}] & \text{for } x \gg 1 \end{cases} \tag{4}$$

and $P_S(\ell, N)$ is normalized according to $\int P_S(\ell, N)\, d\ell = 1$.

Similarly, as for SAWs on regular lattices [18] and on other fractal structures such as Sierpinski triangular lattices [19] and the incipient percolation cluster [8, 10], the exponent δ_S is believed to be given by

$$\delta_S = \frac{1}{1 - \nu_S} \tag{5}$$

while the remaining exponents g_1^S and g_2^S are still unknown. For regular lattices, the corresponding exponent g_1 is given by the des Cloizeaux relation [9]

$$g_1 = \frac{\gamma - 1}{\nu} \tag{6}$$

where the critical exponent γ, describing the total number of SAWs of length N, is denoted as the enhancement exponent (see equation (9) below). For SAWs on the incipient percolation cluster, the modified form (in the Euclidean metric)

$$g_1^r = \frac{\gamma_1 - 1}{\nu_r} + \frac{\beta_{\text{perc}}}{\nu_{\text{perc}}} \tag{7}$$

denoted as the generalized des Cloizeaux relation [10], describes the numerical results very well. Here, β_{perc} and ν_{perc} are the usual critical percolation exponents. The second term has its origin in the disordered nature of the incipient percolation cluster and should not be present for SAWs on deterministic fractals [10]. This conjecture was recently confirmed for SAWs on Sierpinski triangular lattices, for which the simple generalization of equation (6),

$$g_1^{S'} = \frac{\gamma_S' - 1}{\nu_S'} \tag{8}$$

is in very good accordance with the numerical values [19] (ticked quantities such as $g_1^{S'}$, γ_S' and ν_S' refer in the following to the corresponding exponents on Sierpinski triangular lattices). However, as the present study shows, a simple des Cloizeaux relation in the form of equation (8), $g_1^S = (\gamma_S - 1)/\nu_S$, does not hold for Sierpinski square lattices (see the discussion in section 4). Note that only for regular lattices is there an analytical estimate for the exponent g_2, $g_2 = \delta[d(\nu - 1/2) - (\gamma - 1)]$ [20], whereas such a relation is not known for SAWs on fractal structures.

The enhancement exponent γ_S is related to the total number $C_{N,S}$ of SAW configurations of length N on the Sierpinski square lattices by

$$C_{N,S} \sim \mu_S^N N^{\gamma_S - 1} \tag{9}$$

valid for $N \gg 1$, where μ_S is the effective coordination number of Sierpinski square lattices. For SAWs on regular lattices and on the incipient percolation cluster, the corresponding coordination numbers μ and $\mu(p)$ are related by [21]

$$\mu(p) = p\mu \tag{10}$$

where $p \geqslant p_c$ is the percolation occupation probability. It should be emphasized here that the validity of equation (10), for the special case of SAWs on the incipient percolation cluster $p = p_c$, i.e. $\mu(p_c) = p_c\mu$, has been conjectured in [21]. Due to the multifractal nature of SAWs on the incipient percolation cluster [8, 22], however, one needs to study the generalized

coordination numbers $\mu_q(p_c)$, which are related to the (configurational averaged) moments of order q of C_N, $\langle C_N^q \rangle^{1/q}$. These $\mu_q(p_c)$ turn out to vary continuously with q, indicating, in other words, that the results depend on the averaging procedure employed. It has been realized only recently [8] that equation (10) holds for $p = p_c$ in the form $\mu_1 = p_c\mu$, i.e. for the first moment $q = 1$ of the coordination number, while other moments $\mu_q(p_c)$, $q \neq 1$, do not obey equation (10).

One might argue that the validity of equation (10) has its roots in the fact that for SAWs on the percolation clusters, as compared to SAWs on regular lattices, the reduced connectivity of the percolation cluster quantified by the probability p is the dominant issue. Concerning a possible relation between the coordination numbers μ and μ_S for SAWs on regular and on Sierpinski square lattices, respectively, one might argue somewhat differently by assuming that it is not the connectivity of the underlying substrate which is important, but rather the spatial restrictions quantified by the fractal dimension d_f^S of the Sierpinski square lattice. Hence, a relation

$$\mu_S = \frac{d_f^S}{d}\mu \tag{11}$$

seems to be the most natural counterpart of equation (10). This conjecture is obeyed very well in $d = 2$ and $d = 3$, as we discuss later in section 4.

3. Numerical results

To determine the scaling exponents and other quantities as accurately as possible, in particular those characterizing the PDF $P_S(\ell, N)$, an average over different starting points for the SAWs is required to minimize the strong lattice effects typical of Sierpinski structures (see, e.g., [19, 23]). In the case of SAWs on Sierpinski triangular lattices, this averaging method leads to results which compare very well with the values obtained using renormalization group techniques; see table 1 (the quoted values therein are taken from [4, 5, 8–10, 18–20, 24–38]). In the present case, the average is done over 16 starting points in $d = 2$ and 64 in $d = 3$, corresponding to the lattice points of the initiator of the fractal (i.e., of the zeroth iteration step) in both cases. The size of the actual fractal structure and the location of the starting points are chosen such that the generated SAWs cannot reach the boundary (for details of the method employed to guarantee this, see [19]). In what follows, the average over different starting points will be indicated by the symbol $\langle \cdots \rangle$.

3.1. End-to-end chemical distance

The behaviour of the mean end-to-end chemical distance $\langle \overline{\ell}(N) \rangle$ as a function of step length N, obtained by exact enumeration of all walks up to $N = 30$ in $d = 2$ and up to $N = 20$ in $d = 3$, is displayed in figure 2. The insets show the effective exponents $\nu_S(N)$, obtained from the successive slopes $\mathrm{d}\ln\langle\overline{\ell}(N)\rangle/\mathrm{d}\ln N$, plotted as a function of $1/N$. The numerical values of ν_S are reported in table 1. It should be noted that the numerical values obtained for ν_S can hardly be distinguished from the exact values known for the exponent ν for SAWs on regular lattices. Previous investigations in $d = 2$ based on series expansion techniques for $N \leqslant 18$ reported $\nu_S = 0.80 \pm 0.06$ [15]. For consistency, we reanalyse the values of the average square Euclidean end-to-end distance $\overline{r^2}(N)$ given in [15], table IV, using the methods applied here and estimate a somewhat smaller value $\nu_S = 0.77 \pm 0.05$, however consistent with both the previously reported as well as our results. Note that for SAWs on some Sierpinski square

Table 1. An overview of the critical exponents and other quantities for SAWs on various structures. The column 'regular sq/tr' shows the values for regular square/triangular and simple cubic lattices (note that the value for μ is non-universal and depends on the lattice type), 'Sierpinski sq' shows the values for Sierpinski square lattices, 'Sierpinski tr' shows the values for Sierpinski triangular lattices, whereas 'percolation sq' shows the values for the (square lattice) incipient percolation cluster. Note that no sub/superscripts are given in the leftmost column, so that for example the row 'ν' shows ν for regular lattices, ν_{S} for Sierpinski square lattices, ν'_{S} for Sierpinski triangular lattices, and ν_r for the incipient percolation cluster (for the percolation cluster, the values of μ and γ refer to the particular exact enumeration values μ_1 and γ_1 [8], whereas ν, g_1 and g_2 refer to the exponents in the Euclidean metric, ν_r, g_1^r and g_2^r, respectively). Where exact values are given, approximate numerical values are shown in square brackets to ease comparison. For the fractal lattices shown in the three rightmost columns, where known, analytical estimates are given in round brackets to allow an estimation of the accuracy of the numerical values.

		Regular sq/tr	Sierpinski sq	Sierpinski tr	Percolation sq
d_{f}	2D	2	$\ln 8/\ln 3^{\mathrm{a}}$ [≈1.893]	$\ln 3/\ln 2^{\mathrm{b}}$ [≈1.585]	$91/48^{\mathrm{c}}$ [≈1.896]
	3D	3	$\ln 20/\ln 3^{\mathrm{a}}$ [≈2.727]	2^{b}	$2.524 \pm 0.008^{\mathrm{d}}$
ν	2D	$3/4^{\mathrm{e}}$ [=0.75]	0.75 ± 0.05	$0.78 \pm 0.03^{\mathrm{f}}$ (0.798^{g})	$0.787 \pm 0.010^{\mathrm{i}}$
	3D	$7/12^{\mathrm{j}}$ [≈0.583]	0.58 ± 0.03	$0.66 \pm 0.04^{\mathrm{f}}$ (0.674^{h})	$0.662 \pm 0.006^{\mathrm{i}}$
g_1	2D	$11/24^{\mathrm{k}}$ [≈0.458]	0.54 ± 0.03	$0.44 \pm 0.05^{\mathrm{f}}$ (0.47^{l})	$0.55 \pm 0.06^{\mathrm{i}}$ (0.54^{m})
	3D	0.268^{k}	0.16 ± 0.05	$0.65 \pm 0.08^{\mathrm{f}}$ (0.662^{l})	$0.92 \pm 0.08^{\mathrm{i}}$ (0.916^{m})
g_2	2D	$5/8^{\mathrm{n}}$ [=0.625]	1.41 ± 0.08	$2.34 \pm 0.10^{\mathrm{f}}$	$1.56 \pm 0.20^{\mathrm{i}}$
	3D	0.255^{n}	0.10 ± 0.05	$2.6 \pm 0.4^{\mathrm{f}}$	$2.6 \pm 0.2^{\mathrm{i}}$
δ	2D	4^{o}	3.73 ± 0.30 (4^{p})	$5.1 \pm 0.2^{\mathrm{f}}$ (4.965^{p})	$4.85 \pm 0.20^{\mathrm{i}}$ (4.695^{p})
	3D	$12/5^{\mathrm{o}}$ [=2.4]	2.65 ± 0.50 (2.38^{p})	$3.0 \pm 0.3^{\mathrm{f}}$ (3.068^{p})	$3.1 \pm 0.2^{\mathrm{i}}$ (2.960^{p})
μ	2D sq	$2.638\,158\,529\,27\,(1)^{\mathrm{q}}$	2.515 ± 0.015 (2.499^{r})		$1.565 \pm 0.005^{\mathrm{i}}$
	2D tr	$4.150\,96 \pm 0.000\,36^{\mathrm{s}}$		$2.29 \pm 0.01^{\mathrm{f}}$ ($2.288\,03^{\mathrm{t}}$)	
	3D sq	$4.684\,04 \pm 0.000\,09^{\mathrm{u}}$	4.26 ± 0.02 (4.258^{r})		$1.462 \pm 0.005^{\mathrm{i}}$
	3D tr			$3.82 \pm 0.02^{\mathrm{f}}$ (3.815^{v})	
γ	2D	$43/32^{\mathrm{w}}$ [=1.343 75]	1.23 ± 0.04	$1.36 \pm 0.03^{\mathrm{f}}$ (1.3752^{g})	$1.34 \pm 0.05^{\mathrm{i}}$
	3D	$1.1575 \pm 0.0006^{\mathrm{x}}$	1.36 ± 0.03	$1.42 \pm 0.04^{\mathrm{f}}$ (1.4461^{y})	$1.29 \pm 0.05^{\mathrm{i}}$

[a] Obtained by $d_{\mathrm{f}}^{\mathrm{S}} = \ln(n^d - k)/\ln n$.
[b] Obtained by $d_{\mathrm{f}}^{\mathrm{S}'} = \ln(d+1)/\ln 2$.
[c] [24, 25]. [d] [26]. [e] [4]. [f] [19]. [g] [27–30]. [f] [31–33]. [h] [8]. [i] [5]. [j] [9] and equation (6). [k] [19] and equation (8). [l] [10] and equation (7). [m] [20]. [n] [18]. [o] Obtained by equation (5) and its analogues. [p] [34, 35]. [q] Obtained by equation (11). [s] [36]. [t] [27–29]. [u] [37]. [v] [27]. [w] [25]. [x] [38]. [y] [30].

lattices in $d = 2$ characterized by low lacunarity, values for the end-to-end distance exponent smaller than that for the regular square lattices have been reported [15].

3.2. Probability distribution function

Our aim in studying the PDF $P_{\mathrm{S}}(\ell, N)$ for the end-to-end chemical distance, for fixed number of steps N, is to estimate the exponents g_1^{S} and g_2^{S} in both $d = 2$ and $d = 3$. To minimize spurious lattice effects, we study the mean distribution $\langle P_{\mathrm{S}}(\ell, N)\rangle$, averaged over different starting points, as discussed above. The mean PDFs are shown in figure 3. For the Sierpinski square lattices (as well as for other square lattices such as the regular one) one encounters the additional difficulty that for SAWs of odd/even lengths N only odd/even end-to-end distances ℓ can occur due to the lattice topology. Therefore, figure 3 shows the results for both $N = 29$ and $N = 30$ in $d = 2$ and both $N = 19$ and $N = 20$ in $d = 3$. The results of the fits for g_1^{S}, using the asymptotic scaling form equation (4) for $x \ll 1$, are reported in table 1. The second

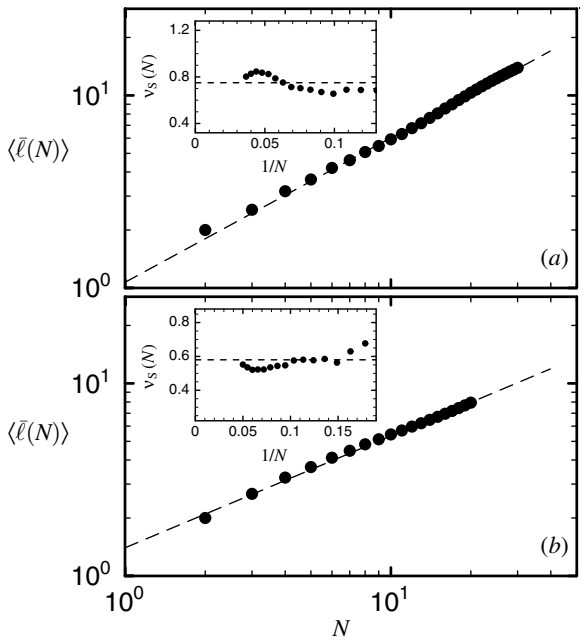

Figure 2. Mean end-to-end chemical distance $\langle\overline{\ell}(N)\rangle$ for SAWs on Sierpinski square lattices as a function of the step length N, using exact enumeration of all walks in the cases: (*a*) $d = 2$ for $N \leqslant 30$, averaged over 16 starting points, and (*b*) $d = 3$ for $N \leqslant 20$, averaged over 64 starting points. The dashed lines display the present results, yielding $\nu_S = 0.75$ ($d = 2$) and $\nu_S = 0.58$ ($d = 3$). The insets show the successive slopes $\nu_S(N) \equiv \mathrm{d}\ln\langle\overline{\ell}(N)\rangle/\mathrm{d}\ln N$ plotted versus $1/N$.

exponent g_2^S is determined by applying a somewhat more sensitive approach, as illustrated in figure 4. The resulting values confirm those obtained directly from figure 3 and are also reported in table 1.

3.3. Total number of SAW configurations

To determine the enhancement exponent γ_S and the effective coordination number μ_S of the Sierpinski square lattices, we studied the total number $\langle C_{N,S}\rangle$ of SAWs of N steps. The behaviour expected from equation (9) is analysed in two different ways, as particularly an accurate determination of γ_S requires a certain care. The first method consists in studying the quantity $\langle C_{N,S}\rangle\mu^{-N}$ as a function of N, for different values of μ, as shown in figure 5. The reported value $\mu = \mu_S$ yields the 'best' power-law dependence of $\langle C_{N,S}\rangle\mu^{-N}$ versus N, for large N. The second method consists in a direct fit of the function $\langle C_{N,S}\rangle = A_S\mu_S^N N^{\gamma_S-1}$ in the form

$$\frac{\ln\langle C_{N,S}\rangle}{N} = \frac{\ln A_S}{N} + \ln\mu_S + (\gamma_S - 1)\frac{\ln N}{N} \tag{12}$$

with suitable values of the fit parameters A_S, γ_S and μ_S. The results are shown in figure 6. Both methods yield consistent results and our final values for γ_S and μ_S are reported in table 1. Previous investigations in $d = 2$ based on series expansion techniques for $N \leqslant 18$ reported $\mu_S = 2.502 \pm 0.003$ and $\gamma_S = 1.35 \pm 0.05$ using a different method of analysis [15]. For consistency, we reanalyse the values of SAW configurations given in [15], table IV, using the methods applied here and estimate $\mu_S = 2.51 \pm 0.02$ and a somewhat smaller

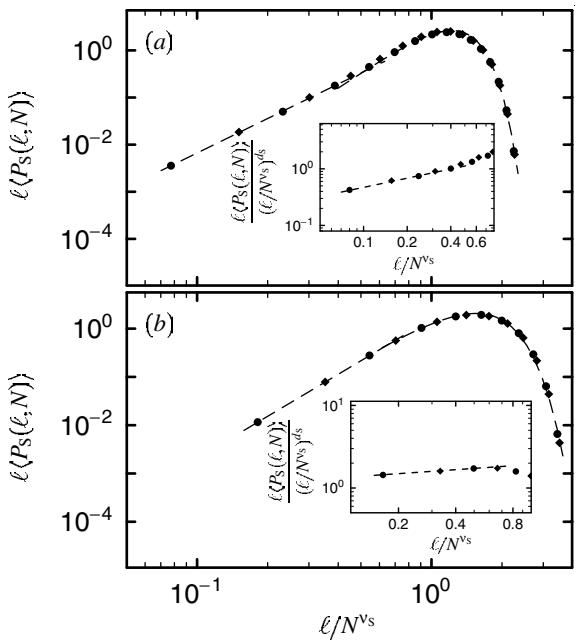

Figure 3. The mean PDF $\langle P_S(\ell, N)\rangle$ for the end-to-end chemical distance ℓ for SAWs of a fixed number of steps N, plotted as $\ell\langle P_S(\ell, N)\rangle$ versus ℓ/N^{ν_S}, in the cases: (*a*) $d = 2$ for $N = 29$ (circles) and 30 (diamonds) using $\nu_S = 0.75$, as well as (*b*) $d = 3$ for $N = 19$ (circles) and 20 (diamonds) using $\nu_S = 0.58$. The dashed lines represent fits of the data, in the regimes $\ell \ll N^{\nu_S}$ and $\ell \gg N^{\nu_S}$, according to equations (3) and (4). (Concerning g_2^S see figure 4.) A more accurate determination of the exponent g_1^S is illustrated in the insets, where the quantity $\ell\langle P_S(\ell, N)\rangle/(\ell/N^{\nu_S})^{d_f^S}$ is plotted versus ℓ/N^{ν_S}. The exponent g_1^S is obtained from the slope of the ansatz $\ell\langle P_S(\ell, N)\rangle/(\ell/N^{\nu_S})^{d_f^S} \sim (\ell/N^{\nu_S})^{g_1^S}$ for $\ell \ll N^{\nu_S}$, yielding the results $g_1^S = 0.54$ in $d = 2$ and $g_1^S = 0.16$ in $d = 3$.

$\gamma_S = 1.28 \pm 0.05$, which is however consistent with both the previously reported as well as our results.

4. Discussion

According to the present results, it appears that SAWs on Sierpinski square lattices display a kind of intermediate behaviour between SAWs on the corresponding regular and Sierpinski triangular lattices (note that such a dependence on the type of underlying Sierpinski structure is also observed for other models, such as Ising models [39]). We summarize our main points as follows:

(i) Structural exponents: ν_S, g_1^S and g_2^S. The exponents describing the structure of SAWs on Sierpinski square lattices behave as their regular counterparts, i.e. ν_S and ν are merely identical for both $d = 2$ and $d = 3$, and g_1^S and g_1 as well as g_2^S and g_2 show the same trend (decrease) with increasing spatial dimension. Furthermore, in both cases the same 'ordering' of the exponents occurs: $g_1 < g_2$ and $g_1^S < g_2^S$ for $d = 2$, but $g_1 > g_2$ and $g_1^S > g_2^S$ for $d = 3$. This has to be distinguished from the behaviour of the corresponding exponents for SAWs on Sierpinski triangular lattices and on the incipient percolation cluster. Here, ν_r and ν_S' are both larger than ν, so that the fractal nature of the underlying

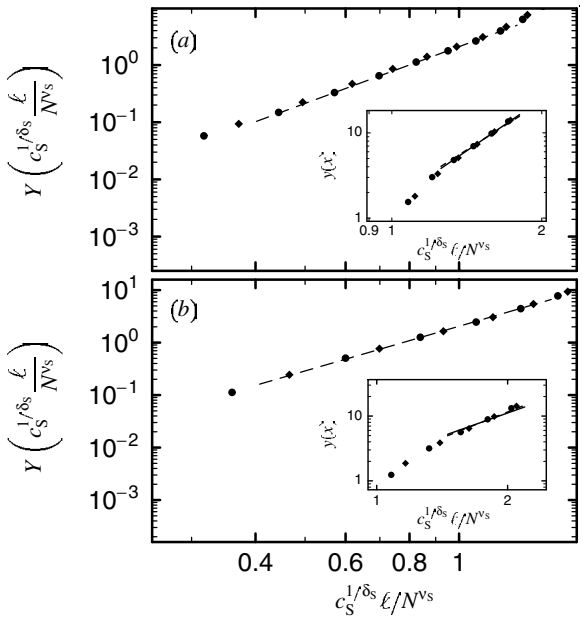

Figure 4. The mean PDF $\langle P_S(\ell, N)\rangle$ for the end-to-end chemical distance ℓ for SAWs of fixed number of steps N, replotting the data of figure 3, for the cases: (*a*) $d = 2$ and (*b*) $d = 3$, analysed according to the method discussed in [8]. Plotted is the quantity $Y(x) \equiv c_S^{(g_2^S+d_f^S)/\delta_S} C_S^{-1}\ell\langle P_S(\ell, N)\rangle \exp[(c_S^{1/\delta_S}\ell/N^{\nu_S})^{\delta_S}]$ versus $x \equiv c_S^{1/\delta_S}\ell/N^{\nu_S}$, which is expected to scale as $Y(x) \sim x^{g_2^S+d_f^S}$. We use $\delta_S = 3.73$ and $c_S = 0.42$ in $d = 2$, and $\delta_S = 2.65$ and $c_S = 0.335$ in $d = 3$ (C_S is a constant related to the normalization of $\langle P_S(\ell, N)\rangle$). The slopes of the dashed lines represent the fitted values of $g_2^S + d_f^S$, yielding the results $g_2^S = 1.41$ in $d = 2$ and $g_2^S = 0.10$ in $d = 3$. The insets show detailed plots to estimate the accuracy of the obtained values of g_2^S. Plotted is the quantity $y(x) \equiv -\ln[C_S^{-1} c_S^{(g_2^S+d_f^S)/\delta_S}\ell\langle P_S(\ell, N)\rangle (c_S^{1/\delta_S}\ell/N^{\nu_S})^{-(g_2^S+d_f^S)}]$ versus $x \equiv c_S^{1/\delta_S}\ell/N^{\nu_S}$, which is expected to scale as $y(x) \sim x^{\delta_S}$, for the values of g_2^S obtained above. The slopes of the dashed lines represent the values of δ_S used above, and the continuous lines represent the values of δ_S obtained by equation (5) using the results for ν_S obtained from figure 2.

lattice is strong enough to affect the spatial structure of the SAWs such that the scaling behaviour changes. Correspondingly, $g_1^{S'}$ and g_1^r as well as $g_2^{S'}$ and g_2^r show the same trend (increase) with increasing spatial dimension. Additionally, the same 'ordering' of the exponents occurs: $g_1^r < g_2^r$ and $g_1^{S'} < g_2^{S'}$ for both $d = 2$ and $d = 3$.

(ii) Configuration space: μ_S and γ_S. The quantities describing the configuration space of SAWs on Sierpinski square lattices behave similarly to their counterparts on Sierpinski triangular lattices, i.e. μ_S and μ'_S increase much more slowly than μ for SAWs on regular lattices; γ_S and γ'_S counterbalance this slow increase and show the same trend (increase) with increasing spatial dimension (suggesting the absence of an upper critical dimension in both cases, see below). This has to be confronted with the behaviour of the corresponding exponents for SAWs on regular lattices and on the incipient percolation cluster, for which the values of γ and γ_1 decrease with increasing spatial dimension, reaching the mean-field value 1 at the upper critical dimension d_c.[4] However, this mean-field behaviour occurs for different reasons. For regular lattices, $\gamma = 1$ for $d = d_c = 4$, as the effect

[4] Note, however, the interesting exact enumeration results for μ and γ of SAWs on a family of Sierpinski triangular lattices which asymptotically approach the regular triangular lattice [40], and the subsequent comment [41].

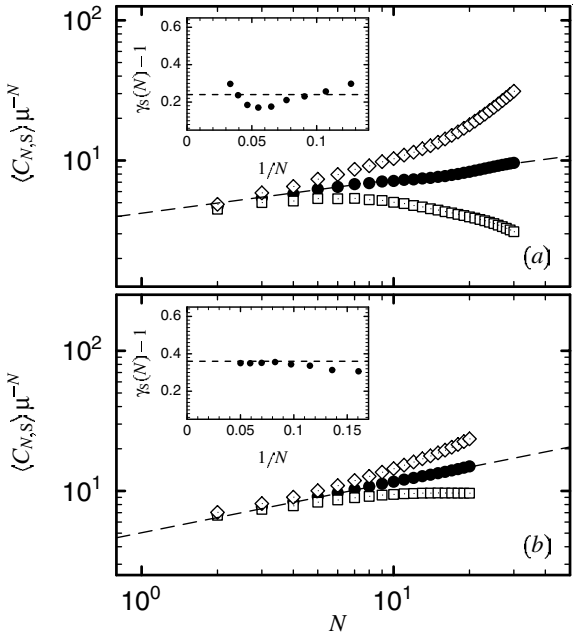

Figure 5. Total number of SAWs of N steps $\langle C_{N,S}\rangle$ on Sierpinski square lattices, plotted as $\langle C_{N,S}\rangle\mu^{-N}$ versus N in double-logarithmic form, for different values of μ. The value for μ_S is obtained when $\langle C_{N,S}\rangle\mu^{-N}$ displays a satisfactory power law, and the associated slope yields $\gamma_S - 1$. The plots correspond to: (*a*) $d = 2$, for $\mu = \mu_S = 2.515$ (circles), $\mu = 2.415$ (diamonds) and $\mu = 2.615$ (squares). The dashed line is a fit yielding $\gamma_S = 1.24$. It is also obtained from the successive slopes $\gamma_S(N) - 1 \equiv \mathrm{d}\ln[\langle C_{N,S}\rangle\mu_S^{-N}]/\mathrm{d}\ln N$ plotted versus $1/N$ in the inset. (*b*) $d = 3$, $\mu = \mu_S = 4.26$ (circles), $\mu = 4.16$ (diamonds) and $\mu = 4.36$ (squares). The successive slopes (inset) yield $\gamma_S = 1.36$, the value is represented by the dashed line.

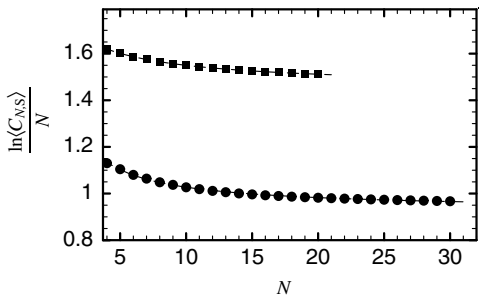

Figure 6. Total number of SAWs of N steps $\langle C_{N,S}\rangle$ on Sierpinski square lattices, plotted as $\ln\langle C_{N,S}\rangle/N$ versus N. The lines are fits using the form $\ln\langle C_{N,S}\rangle/N = (\ln A_S)/N + \ln\mu_S + [(\gamma_S - 1)\ln N]/N$ for $N \geqslant 4$, in $d = 2$ (circles) and $d = 3$ (squares). The resulting values for the fit parameters are $\mu_S = 2.517$, $\gamma_S = 1.22$ and $A_S = 1.7$ in $d = 2$, and $\mu_S = 4.26$, $\gamma_S = 1.36$ and $A_S = 1.2$ in $d = 3$, consistent with those obtained in figure 5.

of self-avoidance of SAWs becomes negligible at the upper critical dimension and SAWs behave as standard random walks, for which $\gamma = 1$. For the incipient percolation cluster, the underlying structure governing the behaviour of the SAWs, which is the percolation backbone, gets less and less compact with increasing spatial dimension, and the topological dimension d_ℓ^{B} of the backbone reaches the value $d_\ell^{\mathrm{B}} = 1$, characteristic of a linear structure, at the upper critical dimension $d_c = 6$. This linear character of

the underlying structure makes the self-avoidance of SAWs irrelevant, so that here also $\gamma_1 = 1$. It seems that for SAWs on Sierpinski square and on Sierpinski triangular lattices, none of these mean-field scenarios occur (see the further discussion concerning upper critical dimensions in point (iv) below).

(iii) Conjecture: μ_S. Based on our results and on values reported previously [15], we propose here relation (11), $\mu_S = \mu d_f/d$, between the coordination numbers μ and μ_S of SAWs on regular square and Sierpinski square lattices, respectively. This relation is fulfilled very accurately: inserting the numerical values summarized in table 1, one obtains $\mu d_f^S/d = 2.499$ in $d = 2$ and 4.258 in $d = 3$, which have to be compared to the numerical values $\mu_S = 2.515$ in $d = 2$ and 4.26 in $d = 3$ obtained from the data shown in figures 5 and 6. Previous results for μ_S for other values of (n, k) in $d = 2$ [15] are also in good accordance with equation (11) and suggest that the proposed relation might hold generally for SAWs on Sierpinski square lattices. Nevertheless, it would be helpful to explore the parameter space of (n, k) in more detail, in particular to study less symmetric arrangements, to further support the conjecture equation (11) with more data. Note that equation (11) holds in any case for the limit of regular square lattices obtained by taking simultaneously $n \to \infty$ and $k \to 0$, as here $d_f^S(n \to \infty, k \to 0) \to d$ and $\mu_S(n \to \infty, k \to 0) \to \mu$ (when simultaneously $n \to \infty$ and $k \to 0$, in particular the symmetric case studied here corresponds asymptotically to regular lattices [42]). The important question whether equation (11) holds in identical or similar form also for SAWs on other deterministic fractals is difficult to answer in general terms, as for example in the case of the Sierpinski triangular lattices, there is no regular counterpart of the fractal structure in $d = 3$ to compare with, and the fractal structure in $d = 2$ uses only at maximum four of six possible connections. Therefore, it is certainly interesting to obtain μ for SAWs on other deterministic fractals which do have a regular counterpart.

(iv) Generalized des Cloizeaux relation: $g_1^S \neq (\gamma_S - 1)/\nu_S$. Due to the intermediate or competing behaviour of SAWs on Sierpinski square lattices sharing aspects of both SAWs on ordered and fractal structures, a des Cloizeaux relation does not hold. One obtains for the naive generalization $(\gamma_S - 1)/\nu_S$ the values 0.32 and 0.62 in $d = 2$ and $d = 3$, respectively, which increase with spatial dimension d. These values have to be compared to the present numerical results $g_1^S = 0.54$ and $g_1^S = 0.16$ in $d = 2$ and $d = 3$, respectively, obtained from figure 3, which decrease with d. Although it is not clear why this competing behaviour occurs, and whether and how the des Cloizeaux relation (6) can be generalized to SAWs on Sierpinski square lattices, we note that the absence of a des Cloizeaux relation might be due to a missing upper critical dimension d_c for SAWs on Sierpinski square lattices. This is suggested by the fact that γ_S *increases* with d. However, an increasing γ_S' with increasing spatial dimension d is also observed for SAWs on Sierpinski triangular lattices [19], and hence the same argument of a missing upper critical dimension also seems to hold true there. Note that in [43] it was predicted for the latter that $\gamma_S' \to 1.618$ for $d \to \infty$, which might indicate, on the other hand, the *existence* of an upper critical dimension d_c (although it might be that $d_c = \infty$). Therefore, the fact that a des Cloizeaux relation holds for SAWs on Sierpinski triangular lattices is not conclusive. The problem whether upper critical dimensions exist might be addressed by investigating the cases $d \geqslant 4$ for both Sierpinski triangular and square lattices, yet such a numerical study is merely impossible with current computers; the values of N that one can manage so far are much too small to give a definite answer.

A second possible direction of further investigation is the construction of deterministic fractal structures which do have an upper critical dimension for SAWs on them. This might

be achieved for instance by studying Sierpinski square lattices and varying the pair (n, k) for various dimensions. One might expect that for large n and small k a 'transition' towards SAWs on regular lattices occurs. As the latter case is characterized by the existence of an upper critical dimension, one obtains deterministic fractal structures sharing this property. An indication of this 'transition' will be that the dependence of γ on the spatial dimension reverses from increasing with d to decreasing with d.

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