A model of compact polymers on a family of three-dimensional fractal lattices

Dušanka Lekić¹ and Sunčica Elezović-Hadžić²

¹ Faculty of Science, Department of Physics, University of Banja Luka, Mladen Stojanovića 2, Banja Luka, Bosnia and Herzegovina
² Faculty of Physics, University of Belgrade, PO Box 44, 11001 Belgrade, Serbia
E-mail: dusamar@netscape.net and suki@ff.bg.ac.rs

Received 15 October 2009
Accepted 22 January 2010
Published 25 February 2010

Abstract. We study Hamiltonian walks (HWs) on the family of three-dimensional modified Sierpinski gasket fractals, as a model for compact polymers in nonhomogeneous media in three dimensions. Each member of this fractal family is labeled with an integer \( b \geq 2 \). We apply an exact recursive method which allows for explicit enumeration of extremely long Hamiltonian walks of different types: closed and open, with end-points anywhere in the lattice, or with one or both ends fixed at the corner sites, as well as some Hamiltonian conformations consisting of two or three strands. Analyzing large sets of data obtained for \( b = 2, 3 \) and 4, we find that numbers \( Z_N \) of Hamiltonian walks, on fractal lattice with \( N \) sites, for \( N \gg 1 \) behave as \( Z_N \sim \omega^N \mu^N \sigma^N \). The leading term \( \omega^N \) is characterized by the value of the connectivity constant \( \omega > 1 \), which depends on \( b \), but not on the type of HW. In contrast to that, the stretched exponential term \( \mu^N \sigma^N \) depends on the type of HW through the constant \( \mu < 1 \), whereas the exponent \( \sigma \) is determined by \( b \) alone. For larger \( b \) values, using some general features of the applied recursive relations, without explicit enumeration of HWs, we argue that the asymptotical behavior of \( Z_N \) should be the same, with \( \sigma = \ln 3 / \ln [b(b + 1)(b + 2)/6] \), valid for all \( b > 2 \). This differs from the formulae obtained recently for Hamiltonian walks on other fractal lattices, as well as from the formula expected for homogeneous lattices. We discuss the possible origins and implications of such a result.

Keywords: solvable lattice models, structures and conformations (theory)

ArXiv ePrint: 0910.2348
1. Introduction

The fact that compact conformations of polymers are principal configurations of the native states of globular proteins makes them an important subset of all the physically accessible conformations. Since compact conformations occupy space as densely as possible, one of the simplest ways to model them is to use Hamiltonian walks (HWs) on a lattice, which are, by definition, self-avoiding walks (SAWs) that visit all the lattice sites exactly once [1]. In order to make this model more capable of capturing different features of various physical phenomena (such as protein melting [2] or protein folding [3]) local interactions can be introduced, but even in its simplest form, with no interactions taken into account, the problem of enumeration and classification of Hamiltonian walks has proved to be extremely difficult.

Studies of Hamiltonian walks are primarily focused on finding the overall numbers $Z_N$ of open and closed HWs on lattices with $N$ sites. It is expected that a limiting value of $\ln Z_N/N$ exists when $N \to \infty$, and its particular value

$$\ln \omega = \lim_{N \to \infty} \frac{\ln Z_N}{N}$$

corresponds to the configurational entropy per monomer (site). This means that to the lowest approximation, $Z_N$ behaves as $\omega^N$ and, therefore, the so-called connectivity constant $\omega > 1$ can be interpreted as the average number of steps available to the walker having already completed a large number of steps. The leading corrections to the exponential term are expected to have the power-law form $N^\alpha$ (as in the case of
ordinary self-avoiding walks), and the stretched exponential form $\mu^N$, with $\mu < 1$, so $Z_N$ should scale as

$$Z_N \sim \omega^N \mu^N N^\sigma.$$  \hspace{1cm} (1.1)

Expectations of such forms are based on the exact studies of HWs on the Manhattan [4] and some fractal lattices [5]–[7], as well as on results obtained for closely related models of collapsed interacting self-avoiding walks on square [8]–[11] and cubic lattices [12]. In the case of collapsed SAWs the appearance of the stretched exponential term, which is not present in the scaling form for non-interacting SAWs, was explained as a consequence of surface effects. Namely, a collapsed SAW forms a compact globule, with a sharp boundary separating it from the surrounding solvent, so monomers on the boundary have a smaller number of contacts with other monomers than those in the bulk of the globule, and therefore surface tension should arise. For homogeneous lattices one can assume that the boundary itself is a homogeneous surface, and then straightforward arguments [13] lead to the conclusion that the term $\mu^N$, with $\sigma = (d-1)/d$ ($d$ being the dimensionality of the lattice), should appear. Exact studies [9], series analysis of data obtained via exact enumeration [8,10], as well as Monte Carlo simulations [11,12] of collapsed SAWs on homogeneous lattices certainly confirm the existence of the stretched exponential term with the proposed formula for $\sigma$. Although it is believed that the HW model corresponds to the interacting SAW model at temperature $T = 0$, in spite of the continuous improvements of exact [14] and Monte Carlo [15] enumeration techniques, direct confirmation of the scaling relation (1.1) for HWs on non-oriented homogeneous lattices has not been achieved yet. Other than for the Manhattan lattice, scaling forms for Hamiltonian walks have been obtained only for some fractal lattices, where stretched exponential corrections for both open and closed HWs were found only for $n$-simplex fractals with even $n$ [7]. Even in that case, its presence cannot be explained using a simple generalization of the argument used for collapsed self-avoiding walks on homogeneous lattices. However, results of the studies on fractals suggest that a stretched exponential term can be expected for lattices where a larger number of entangled conformations is possible. In order to get a deeper insight into this issue, here we apply an exact recursive method for enumeration and classification of HWs on the modified three-dimensional Sierpinski gasket family of fractals. In contrast to most of the fractals studied previously in this context, which were embedded either in two-dimensional spaces or spaces with dimensionality higher than 3, each member of the family studied in the present paper is embedded in three-dimensional space. Therefore, HWs on these fractals can be understood as a toy model for compact polymer critical behavior in realistic nonhomogeneous 3D media, which, to the best of our knowledge, has not been studied so far.

The paper is organized as follows. Modified 3D Sierpinski gasket fractals, as well as the method itself, are described in section 2. Explicit forms of the recursion relations, obtained for the kinds of Hamiltonian walks which are needed for generation and enumeration of all closed conformations are presented for the first three members of the fractal family. Numerically analyzing these relations, we find the scaling form $\omega^N \mu^N$. Using some general features of these relations (obtained in appendices A and B), we argue that such a form should be correct for the whole fractal family, and derive the closed-form formula for the exponent $\sigma$. In section 3 we extend the method to open HWs, explicitly apply it again to the first three fractals, and then generalize it. It turns out that the number of open HWs
2. Closed Hamiltonian walks on modified three-dimensional Sierpinski gaskets

A three-dimensional modified Sierpinski gasket (3D MSG) fractal is constructed recursively, starting with a unit tetrahedron. The first step of the construction, the so-called generator $G_1(b)$ of order $l = 1$, is obtained by joining

$$N_G = b(b+1)(b+2)/6$$

unit tetrahedrons into a tetrahedral structure $b$ times larger (see figure 1) in such a way that vertices of neighboring unit tetrahedrons are connected via infinitesimal junctions. Enlarging the generator $b$ times, and replacing the smallest tetrahedrons with $G_1(b)$, and then repeating this procedure $l$ times, one obtains $G_{l+1}(b)$—the generator of order $l + 1$, which contains $N_{l+1} = 4N_G^{l+1}$ sites. The complete 3D MSG fractal with parameter $b$ is obtained when $l \to \infty$, and its fractal dimension $d_f$ is equal to

$$d_f = \ln[b(b+1)(b+2)/6]/\ln b.$$  

One should note here that the ordinary 3D Sierpinski gasket (SG) fractal with parameter $b$ is constructed in a similar way, with the only difference being that neighboring unit tetrahedrons in the 3D SG lattice are not moved apart, as is the case for the 3D MSG fractal. This small change does not alter the basic properties of the lattice, such as its fractal dimension, but it simplifies the complicated scheme needed for enumeration of closed Hamiltonian walks on 3D SG fractals [6] and allows for enumeration of extremely long open HWs on 3D MSG fractals with $b = 2, 3,$ and 4. In addition, general conclusions...
A model of compact polymers on a family of three-dimensional fractal lattices

Figure 2. Example of a closed Hamiltonian walk (red line) on the generator of the 3D $b = 3$ MSG fractal. The generator consists of 40 vertices, which are numbered consecutively from the first (arbitrarily chosen) vertex visited by the HW to the last one (which is connected to the first one). One can note that the HW conformation within the unit tetrahedron can be either one-stranded ($B$ type), like the one connecting the sites 26–27–28–29, or two-stranded ($E$ type), like the conformation traversing the tetrahedron with vertices 4–5–12–13.

as regards scaling forms of the numbers of HWs on a 3D MSG fractal with arbitrary $b > 2$ can be derived, as will be explained in what follows.

By definition, each Hamiltonian walk on a $G_l(b)$ structure visits all of its $N_l$ sites exactly once. In figure 2 an example of a closed Hamiltonian walk on the generator $G_1(3)$ is shown. One can note that this HW can be decomposed into $N_G = 10$ parts (within the ten unit tetrahedrons), which are either one-stranded or two-stranded. This observation can easily be generalized to generators of higher order and any $b$: any closed HW on $G_l+1(b)$ can be decomposed into $N_G$ parts within the same number of generators $G_l(b)$, from which the generator $G_l+1(b)$ is made. These parts traverse each $G_l(b)$ either once or two times, and we shall call the corresponding configurations $B$- or $E$-type HW steps, respectively, whereas numbers of HWs of these types within a $G_l(b)$ will be denoted by $B_l$ and $E_l$, respectively. Using these numbers, the overall number of closed HWs on $G_l+1(b)$ can be expressed as

$$Z^C_{l+1} = \sum_{k=0}^{k_C} n_k B_l^{N_G-k} E_l^k,$$

(2.3)

where $n_k$ are the numbers of closed HWs configurations within $G_l+1(b)$, with $k$ steps of $E$ type, and $(N_G-k)$ $B$-type steps. For instance, the path presented in figure 2 is one of $Z^C_1$ possible closed HWs within $G_1(3)$, contributing to the term $n_2 B_0^8 E_1^2$ in the corresponding equation (2.3). The upper limit $k_C$ in the sum in (2.3) is equal to 0 for $b = 2$, whereas for $b > 2$ it can be shown (see appendix A) that

$$k_C = \frac{1}{2}(b+1)(b+2) - 8.$$

(2.4)
A model of compact polymers on a family of three-dimensional fractal lattices

Table 1. Coefficients appearing in recursion relations (2.5), found by direct computer enumeration of the corresponding HW conformations on 3D MSG fractals with \( b = 2, 3, 4 \).

| \( b = 2 \) | \( b = 3 \) | \( b = 4 \) |
|---|---|---|
| \( k \) | \( m_k \) | \( p_k \) | \( k \) | \( m_k \) | \( p_k \) | \( k \) | \( m_k \) | \( p_k \) |
| 0 | — | 22 | 2 | — | 4308 | 7 | — | 26465392 |
| 1 | — | 0 | 3 | — | 1936 | 8 | — | 99652120 |
| 2 | 6 | 0 | 4 | — | 5808 | 9 | — | 151443088 |
| 3 | 4 | 4 | 5 | 3192 | 1888 | 10 | 23848720 | 199987864 |
| 4 | 2 | 1 | 6 | 848 | 2534 | 11 | 58605536 | 204194352 |
| — | — | — | 7 | 1728 | 1056 | 12 | 78351952 | 172479256 |
| — | — | — | 8 | 664 | 596 | 13 | 81469824 | 126633376 |
| — | — | — | 9 | 332 | 160 | 14 | 66418856 | 78454776 |
| — | — | — | 10 | 64 | 32 | 15 | 43526336 | 41200784 |
| — | — | — | — | — | — | 16 | 22989024 | 18548660 |
| — | — | — | — | — | — | 17 | 9642816 | 1001008 |
| — | — | — | — | — | — | 18 | 3032724 | 1901008 |
| — | — | — | — | — | — | 19 | 626056 | 397392 |
| — | — | — | — | — | — | 20 | 62434 | 42514 |

Due to the self-similarity of the lattices under study, the numbers \( n_k \) do not depend on \( l \), and, also, the numbers \( B_l \) and \( E_l \) fulfill recursion relations of the following form:

\[
B_{l+1} = \sum_{k=k_B}^{N_G} m_k B_l^k E_l^{N_G-k}, \quad E_{l+1} = \sum_{k=k_E}^{N_G} p_k B_l^k E_l^{N_G-k}, \tag{2.5}
\]

where coefficients \( m_k \) and \( p_k \) depend only on \( k \) and \( b \), and are positive integers for all \( b > 2 \), including zero for \( b = 2 \). For instance, for \( b = 2 \) these relations are \(^3\)

\[
B_{l+1} = 2B_l^4 + 4B_l^3 E_l + 6B_l^2 E_l^2, \quad E_{l+1} = B_l^4 + 4B_l^3 E_l + 22E_l^4, \tag{2.6}
\]

and we were able to find the explicit form of relations (2.5) for \( b = 3 \) and 4 also, by direct computer enumeration of possible HW conformations within the MSG generator. The corresponding coefficients \( m_k \) and \( p_k \) are presented in table 1, while for larger \( b \) values they could not be reached within a reasonable time with the computer facilities available to us. However, one can show (see appendix A) that for general \( b > 2 \) the lower limits of the sums in relations (2.5) are equal to

\[
k_B = N_G - k_C - 3 = \frac{1}{6} (b + 1)(b + 2)(b - 3) + 5, \quad k_E = k_B - 3, \tag{2.7}
\]

which is a result essential for establishing some general conclusions, as will be explained in the following paragraphs.

Once the explicit form of recursion relations (2.3) and (2.5) is established, starting with the initial values \( B_0 = 2 \), and \( E_0 = 1 \), corresponding to the unit tetrahedron, one can calculate the numbers \( B_l, E_l \), and subsequently the overall number \( Z_{l+1}^C \) of closed HWs, in principle for any \( l \). However, since these numbers quickly become extremely large, it

\(^3\) Note that for \( b = 2 \), recursion relations (2.5) are the same as for the 4-simplex fractal lattice [5].

doi:10.1088/1742-5468/2010/02/P02021
Table 2. Values of relevant constants appearing in the scaling forms (2.17) and (3.13) of the overall numbers of HWs on 3D MSG fractals, with \(b = 2, 3, 4\), together with the corresponding values of the fractal dimension \(d_f\).

| \(b\) | \(d_f\) | \(k_C\) | \(\lambda\) | \(\omega\) | \(\mu_C\) | \(\mu_\sigma\) | \(\sigma\) | \(1/d_f\) |
|------|--------|-------|-------|-------|-------|-------|-------|-------|
| 2    | \(\ln 4/\ln 2\) | 0     | 0.8366| 1.0876| 0.8366| 0.9147| 0.5   | 0.5   |
| 3    | \(\ln 10/\ln 3\) | 2     | 0.8835| 1.4404| 0.8963| 0.9554| 0.4471| 0.4471|
| 4    | \(\ln 20/\ln 4\) | 7     | 0.8639| 1.4686| 0.8696| 0.9496| 0.3667| 0.4628|

is useful to introduce the new variable \(x_l = B_l/E_l\). Then, from (2.5) it follows that the recursion relation for the variable \(x_l\), for \(b > 2\), has the form

\[
x_{l+1} = x_l^{k_B-k_E} g(x_l) = x_l^3 g(x_l), \quad g(x) = \frac{\sum_{k=0}^{k_C+3} m_{k_B} x^k}{\sum_{k=0}^{k_C+6} p_{k_E} x^k}. \tag{2.8}
\]

Numerical analysis of this recursion relation for the \(b = 3\) and \(4\) cases shows that starting with the initial value \(x_0 = 2\), \(x_l\) quickly tends to 0 as \(l\) grows. Assuming that this is correct for general \(b > 2\), for large values of \(l\) the above equation can be approximated as

\[
x_{l+1} \approx \frac{m_{k_B}}{p_{k_E}} x_l^3, \tag{2.9}
\]

from which

\[
x_l \sim \lambda^{3l} \tag{2.10}
\]

follows, where \(\lambda\) is some constant, whose value depends on \(b\), but it is always less than 1. For \(b = 2\) the corresponding relation is \(x_l \sim \lambda^{2l}\) [5], and particular values of \(\lambda\) for the \(b = 2, 3\) and \(4\) cases are given in Table 2.

The recursion relation for numbers \(E_l\) of two-stranded HWs (2.5) with the variable \(x_l = B_l/E_l\) takes the form

\[
E_{l+1} = E_l^{N_G} x_l^{k_B} f(x_l), \quad f(x) = \sum_{k=0}^{k_C+6} p_{k+k_E} x^k, \tag{2.11}
\]

from which one gets

\[
\frac{\ln E_{l+1}}{4N_G^{l+1}} = \frac{\ln E_l}{4N_G^l} + k_E \frac{\ln x_l}{4N_G^{l+1}} + \frac{\ln f(x_l)}{4N_G^{l+1}}. \tag{2.12}
\]

Numerically iterating this recursion relation, together with (2.8), one finds that

\[
\lim_{l \to \infty} \frac{\ln E_l}{4N_G^l} = \ln \omega, \tag{2.13}
\]

where \(\omega\) (see Table 2) is a constant larger than 1. On the other hand, the overall number \(Z_{l+1}^C\) (2.3) of closed HWs on the generator of order \(l + 1\) can be expressed as

\[
Z_{l+1}^C = E_l^{N_G} x_l^{N_G-k_C} h(x_l), \quad h(x) = \sum_{k=0}^{k_C} n_{k_C-k} x^k, \tag{2.14}
\]

\(^4\) The corresponding analysis of the \(b = 2\) case is the same as for the 4-simplex fractal lattice, which is given in [5].

doi:10.1088/1742-5468/2010/02/P02021
A model of compact polymers on a family of three-dimensional fractal lattices

and so

\[
\frac{\ln Z_{l+1}^C}{4N_{l+1}^G} = \frac{\ln E_l}{4N_l^G} + \frac{N_G - k_C \ln x_l}{4N_G} + \frac{\ln h(x_l)}{4N_l^G}. \tag{2.15}
\]

From the asymptotical behavior (2.10) of the number \(x_l\), and from the fact that \(h(x)\) tends to the constant value \(n_{k_C} > 0\) when \(x \to 0\), it then follows that

\[
\lim_{l \to \infty} \frac{\ln Z_l^C}{N_l} = \lim_{l \to \infty} \frac{\ln E_l}{4N_l^G} = \ln \omega,
\]

where \(N_l = 4N_G^l\) is the overall number of vertices within the generator of order \(l\).

To find the leading-order correction to the asymptotic behavior of \(Z_l^C\) we first introduce the variable

\[
y_l = \frac{\ln E_l}{4N_l^G} = \ln \frac{E_l}{N_l}, \tag{2.16}
\]

which, as follows from (2.12), satisfies the relation

\[
y_l = \sum_{k=0}^{l-1} (y_{k+1} - y_k) + y_0 = \sum_{k=0}^{l-1} \frac{1}{N_{k+1}} [k_E \ln x_k + \ln f(x_k)].
\]

Then, using (2.13), one obtains

\[
y_l = \ln \omega - \sum_{k=1}^{\infty} \frac{1}{N_{k+1}} [k_E \ln x_k + \ln f(x_k)],
\]

from which, taking into account the large \(k\) behavior (2.10) of \(x_k\), it follows that

\[
y_l \approx \ln \omega - \frac{1}{N_l N_G - 3} 3^l \ln \lambda - \frac{\text{const}}{N_l}, \quad l \gg 1.
\]

Substituting this relation into (2.15) one derives

\[
\ln Z_l^C \approx N_l \ln \omega + N_l^2 \ln \mu_C, \quad \text{i.e.} \quad Z_l^C \sim \omega^{N_l} \mu_C^{N_l^2}, \tag{2.17}
\]

with

\[
\sigma = \frac{\ln 3}{\ln N_G} = \frac{\ln 3}{\ln[b(b+1)(b+2)/6]^l}, \tag{2.18}
\]

and

\[
\mu_C = \lambda^A, \quad A = \frac{N_G + k_C}{N_G - 3} 4^{-\sigma}. \tag{2.19}
\]

At the end of this section we want to emphasize that the crucial step in preceding derivation, which led to the scaling form (2.17), with the value of the exponent \(\sigma\) given by formula (2.18), was the assumption that \(x_l\) tends to 0 for general \(b\) (explicitly confirmed only up to \(b = 4\)). Its direct consequence is the approximate difference equation (2.9), which is obtained from the exact relation (2.8). On the other hand, the key ingredient of that relation is the fact that \(k_B - k_E = 3\), due to which \(x_l\) behaves as \(\lambda^3\), for \(l \gg 1\). In that sense, exact expressions for \(k_B\) and \(k_E\) (2.7), obtained in appendix A for general \(b > 2\), are essential for establishing the scaling form (2.17), whereas the particular values
A model of compact polymers on a family of three-dimensional fractal lattices

Figure 3. Three examples of open HWs (oriented red lines, where the only meaning of the arrows is to serve as guides to the eye) on the generator of the 3D $b = 3$ MSG fractal. Points at which the HW begins or terminates are marked as full red circles, for the sake of better recognition. If both ends of the walk are in the same tetrahedron the two-leg HW conformation within that tetrahedron is either of $D$ type or $H$ type. Otherwise, if end-points of the walk belong to different tetrahedrons, the corresponding one-leg conformations are of $A$ type or $C$ type.

of the coefficients $m_k$ and $p_k$ of the recursion relations (2.5) do not affect either its general form or the value of $\sigma$. However, whether $x_l$ tends to 0 or not certainly depends on the values of $m_k$ and $p_k$. Analyzing data given in table 1 for $b = 3$ and 4, one can observe that $p_{kE+k} > m_{kE+k+1}$ for $2 \leq k \leq k_C + 5$. It can be shown (see appendix B) that such an inequality for general $b > 2$ is sufficient for proving that the numbers $x_l$, which satisfy difference equation (2.8) with the initial condition $x_0 = 2$, tend to 0 when $l \to \infty$. Unfortunately, we were not able to prove the inequality itself, but since it seems plausible, we think that the scaling relation (2.17) can be accepted as valid for general $b$.

3. Open Hamiltonian walks on modified three-dimensional Sierpinski gaskets

Any open HW on a generator $G_{l+1}(b)$ of order $l + 1$ can be decomposed into $N_G$ parts within its $N_G$ constitutive generators $G_l(b)$ of order $l$. The parts which contain ending points (see figure 3) can be of four different types:

- $A$ type, which consists of one HW, with one end at one vertex of $G_l(b)$ and the other end at any other site of $G_l(b)$, including its vertices;
A model of compact polymers on a family of three-dimensional fractal lattices

- $C$ type, composed of two non-intersecting SAWs, one with both ends at the vertices of the $G_i(b)$, and the other with one end at the third vertex of the $G_i(b)$ and the second anywhere within it—these two SAWs together visit all the sites of the $G_i(b)$;
- $D$ type, consisting of two non-intersecting SAWs, each of them starting at a different vertex of $G_i(b)$ and ending anywhere within it, in such a way that all sites of $G_i(b)$ are visited;
- $H$ type, comprised of three non-intersecting SAWs, each of them starting at a different vertex of $G_i(b)$, one ending at the fourth vertex, and the remaining two anywhere within $G_i(b)$—again, all sites of $G_i(b)$ should be visited by these three SAWs.

$A$- and $C$-type configurations have one dangling end; therefore we shall call them one-leg configurations (steps), whereas $D$- and $H$-configurations, with two dangling ends, will be called two-leg steps. If both end-points of the complete HW lie in the same $G_i(b)$, that $G_i(b)$ contains a two-leg step (of $D$ type or $H$ type), whereas the remaining $N_G - 1$ generators $G_i(b)$ contain either a $B$-step or an $E$-step. Otherwise, when end-points are in two different $G_i(b)$ generators, the complete open HW has two one-leg steps (of $A$ type or $C$ type), and the remaining $N_G - 2$ parts of the walk are of either $B$ type or $E$ type. Therefore, one concludes that overall number $Z^O_{i+1}$ of open HWs within $G_{i+1}(b)$ is equal to

$$Z^O_{i+1} = A_i^2 F_{AA} + A_i C_i F_{AC} + C_i^2 F_{CC} + D_i S_D + H_i S_H,$$

where $F_{AA}$, $F_{AC}$, $F_{CC}$, $S_D$ and $S_H$ are polynomials in $B_i$ and $E_i$, of power $N_G - 2$ or $N_G - 1$, and $A_i$, $C_i$, $D_i$ and $H_i$ are overall numbers of corresponding HW types within the $G_i(b)$ generator. Numbers of one-leg conformations fulfill recursion relations of the following form:

$$A_{i+1} = R_{11}(B_i, E_i) A_i + R_{12}(B_i, E_i) C_i,$$
$$C_{i+1} = R_{21}(B_i, E_i) A_i + R_{22}(B_i, E_i) C_i,$$

with

$$R_{ij}(B, E) = \sum_{k=0}^{k_{ij}} t_{ij}^{k} B^{N_G - 1 - k} E^{k},$$

while numbers of two-leg conformations obey relations of the form

$$D_{i+1} = d_D D_i + d_H H_i + d_{AA} A_i^2 + d_{AC} A_i C_i + d_{CC} C_i^2,$$
$$H_{i+1} = h_D D_i + h_H H_i + h_{AA} A_i^2 + h_{AC} A_i C_i + h_{CC} C_i^2,$$

with $d$ and $h$ being some polynomials in $B_i$ and $E_i$. For instance, for $b = 2$, relations (3.1) and (3.2) are

$$Z^O_{i+1} = 12B_i^3(A_i^2 + 2A_i C_i + 3C_i^2 + B_i D_i),$$
$$A_{i+1} = (6B_i^3 + 6B_i^2 E_i) A_i + (12B_i^3 + 18B_i^2 E_i) C_i,$$
$$C_{i+1} = (B_i^3 + 3B_i^2 E_i) A_i + (3B_i^3 + 12B_i^2 E_i + 16B_i E_i^2 + 16E_i^3) C_i.$$

They coincide with the corresponding relations for the 4-simplex fractal lattice, as does the complete further analysis, which can be seen in [7]. In the remaining part of this section we present the general analysis for $b > 2$ 3D MSG fractals.
For general $b > 2$ it can be shown (see appendix C) that polynomials $F$ and $S$, appearing in (3.1), have the form

$$F_{XY}(B, E) = \sum_{k=0}^{k_C+1} z^X_k B^{N_C-k-2} E^k, \quad XY = AA, AC, CC$$

$$S_D(B, E) = \sum_{k=0}^{k_C} z^D_k B^{N_C-k-1} E^k, \quad S_H(B, E) = \sum_{k=0}^{k_C-1} z^H_k B^{N_C-k-1} E^k. \quad (3.5)$$

Starting with the initial values for the numbers $B_l, E_l, A_l, C_l, D_l, H_l$, and using the recursive relations (2.5), (3.2), and (3.4), one can calculate these numbers in principle for any $l$, and substituting them into (3.1), eventually find the overall number $Z^{O}_{l+1}$ of open HWs. Since all of these numbers increase rapidly with $l$, it is useful to introduce the variables

$$u_l = \frac{A_l}{E_l}, \quad v_l = \frac{C_l}{E_l}, \quad w_l = \frac{D_l}{E_l}, \quad q_l = \frac{H_l}{E_l}, \quad (3.6)$$

in addition to already defined $x_l = B_l/E_l$. With these variables, $Z^{O}_{l+1}$ can be rewritten as

$$Z^{O}_{l+1} = E_l^{N_C} x_l^{N_C-k_C-3} \sum_{k=0}^{k_C+1} \left( \sum_{k_{C+1}}^{k_C} (z^A_{k_{C+1}} u^2_l + z^A_{k_{C+1}} u_l v_l + z^C_{k_{C+1}} v^2_l) x^k_l \right)$$

$$+ w_l x^2_l \sum_{k=0}^{k_C} z^D_{k_{C}-k} x^k_l + q_l x^2_l \sum_{k=0}^{k_C-1} z^H_{k_{C}-k-1} x^k_l, \quad (3.7)$$

and explicitly calculated using corresponding recursion relations for $u_l, v_l, w_l$, and $q_l$, simultaneously with (2.8) and (2.11). In appendix C it is shown that the upper limits of the sums in (3.3) are equal to

$$k_{11} = k_{12} = k_C + 2, \quad k_{21} = k_{22} = k_C + 5, \quad (3.8)$$

and so by dividing (3.2) by the recursion relation for $E_l$, given in (2.5), for $u_l$ and $v_l$ one obtains the recursion relations

$$\begin{pmatrix} u_{l+1} \\ v_{l+1} \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} u_l \\ v_l \end{pmatrix}, \quad (3.9)$$

where the $m_{ij}$ are functions of $x_l$ of the following form:

$$m_{1i}(x) = \frac{x^3}{f(x)} \sum_{k=0}^{k_C+2} r^{1i}_{k_C+2-k} x^k, \quad m_{2i}(x) = \frac{1}{f(x)} \sum_{k=0}^{k_C+5} r^{2i}_{k_C+5-k} x^k, \quad i = 1, 2,$$

and $f(x)$ is defined in (2.11). Since $x_l \rightarrow 0$ and $f(x_l) \rightarrow \text{const} \neq 0$ when $l \rightarrow \infty$, it follows that $m_{1i}(x_l) \rightarrow 0, m_{2i}(x_l) \rightarrow \text{const} \neq 0$, implying that $u_l$ tends to 0, and $v_l$ to some constant value. This is indeed correct for the $b = 3$ and 4 cases, for which we managed to find the complete set of coefficients $r^{ij}_k$ (see table 3). Starting with the initial values $A_0 = 6, C_0 = 2$, i.e. $u_0 = 6$ and $v_0 = 2$, and numerically iterating relations (3.9), for both $b = 3$ and 4, after five iterations one already obtains limiting values of $v_l$: 441.32· for $b = 3$, and 3538.91· for $b = 4$. 

doi:10.1088/1742-5468/2010/02/P02021
In appendix D it is shown that recursion relations for the variables $w_l$ and $q_l$ can be put into the following matrix form:

$$
\begin{pmatrix}
  w_{l+1} \\
  q_{l+1}
\end{pmatrix} = \begin{pmatrix}
  p_{11} & p_{12} \\
  p_{21} & p_{22}
\end{pmatrix} \begin{pmatrix}
  w_l \\
  q_l
\end{pmatrix} + \begin{pmatrix}
  t_{11}u_l^2 + t_{12}u_lv_l + t_{13}v_l^2 \\
  t_{21}u_l^2 + t_{22}u_lv_l + t_{23}v_l^2
\end{pmatrix},
$$

where $p_{ij}$ and $t_{ij}$ are functions of $x_l$ of the form

$$
\begin{align*}
p_{11}(x) &= \frac{x^2}{f(x)} \sum_{k=0}^{kC+3} (k + k_B)m_{k+kB}x^k, \\
p_{12}(x) &= \frac{2x^3}{f(x)} \sum_{k=0}^{kC+2} (kC + 3 - k)m_{k+kB}x^k, \\
p_{21}(x) &= \frac{1}{2x^2f(x)} \sum_{k=0}^{kC+6} (k + k_E)p_{k+kE}x^k, \\
p_{22}(x) &= \frac{1}{f(x)} \sum_{k=0}^{kC+6} (kC + 6 - k)p_{k+kE}x^k, \\
t_{11}(x) &= \frac{1}{f(x)} \sum_{k=0}^{kC+4} s_{kC+4-k}x^k, \\
t_{21}(x) &= \frac{1}{x^3f(x)} \sum_{k=0}^{kC+7} o_{kC+7-k}^A x^k, \\
t_{22}(x) &= \frac{1}{x^2f(x)} \sum_{k=0}^{kC+5} o_{kC+5-k}^{AC} x^k, \\
t_{23}(x) &= \frac{1}{x^3f(x)} \sum_{k=0}^{kC+5} o_{kC+5-k}^{CC} x^k,
\end{align*}
$$

with $s_{kC}$ and $o_{kC}^{XY}$ being some positive constant integers. Using these relations, one can calculate $w_l$ and $q_l$, and by putting them, together with $x_l$, $u_l$, $v_l$ and $E_l$, into (3.7), one can finally evaluate $Z_l^O$, for any $l$.

In order to find the asymptotic behavior of $Z_l^O$, we first notice that relations (3.10) can be combined with the relation (2.8) for $x_l$, so one can establish recursion relations for $w_lx_l^2$ and $qx_l^3$, terms through which variables $w_l$ and $q_l$ appear in (3.7). Using the facts
that \( x_l \to 0 \), \( f(x_l) \to p_{kx} \), \( u_l \to 0 \), and \( v_l \to \text{const.} \), when \( l \to \infty \), it can be shown that

\[
(w_l x_l^2)_{l+1} \approx x_l^6 \left[ \left( \frac{a_{11}}{a_{22}} \right) \left( \frac{w_l x_l^2}{q_l x_l^3} \right) + \left( \frac{b_{i3} v_l^2}{0} \right) \right], \tag{3.12}
\]

where \( a_{ij} \) and \( b_{i3} \) are some constants (see appendix D). This relation implies that \( w_l x_l^2 \) and \( q_l x_l^3 \) tend to zero as \( l \to \infty \), and consequently, comparing the terms containing \( w_l x_l^2 \) and \( q_l x_l^3 \) with those with \( u_l \) and \( v_l \) in (3.7), one can conclude that

\[
Z_{l+1}^O \approx E_l^{NG} x_l^{N_G-k_c-3} \sum_{k=0}^{k_c+1} \left( z_{k_{c+1-k} u_l^2}^{AA} + z_{k_{c+1-k} u_l v_l}^{AC} + z_{k_{c+1-k} v_l^2}^{CC} \right) x_l^k.
\]

This means that for \( l \gg 1 \) the number \( Z_{l+1}^O \) behaves as

\[
Z_{l+1}^O \sim E_l^{NG} x_l^{N_G-k_c-3},
\]

and so, using (2.14), one obtains

\[
\frac{Z_{l+1}^O}{Z_{l+1}^C} \sim x_l^{-3} \sim \lambda^{-3l+1}.
\]

Consequently, taking into account (2.17), it follows that the overall number \( Z_l^O \) of open HWs scales as

\[
Z_l^O \sim \omega^N_{l} \mu_O^{N_{l}}, \quad \mu_O = \lambda^B, \quad B = \frac{k_c + 3}{N_G - 3} 4^{-\sigma}, \tag{3.13}
\]

where, as in (2.18), \( \sigma = \ln 3/\ln N_G \), and particular values of \( \omega, \mu_O \) and \( \lambda \) are given in table 2.

4. Summary and discussion

In this paper we have analyzed the asymptotic behavior of the numbers of open and closed Hamiltonian walks on the three-dimensional modified Sierpinski gasket family of fractals. Numbers of extremely long HWs on these lattices can be generated by applying an exact recursive enumeration scheme, based on the fact that any HW on the \((l+1)\) th step of the construction of the 3D MSG fractal, \( G_{l+1}(b) \), consists of \( N_G = b(b+1)(b+2)/6 \) HWs within its \( N_G \) constitutive \( G_l(b) \) structures, which can be of one of six possible types: \( A, B, C, D, E, \) and \( H \) (figures 2 and 3). Numbers of these HWs, \( A_l, B_l, C_l, D_l, E_l, \) and \( H_l \), fulfill a closed set of recursive relations, (2.5), (3.2) and (3.4), which, due to the self-similarity of the lattices under study, do not depend on \( l \), and therefore can be obtained by explicit enumeration and classification of HW conformations on the first step of the fractal construction, \( G_1(b) \). As \( b \) grows, the number of HW conformations rapidly increases already on \( G_1(b) \), so we have managed to find explicit forms of the recursive relations only up to \( b = 4 \). However, we have shown that for any \( b > 2 \) these recursive relations have some features that enable general analysis, leading to the conclusion that overall numbers \( Z_l^C \) and \( Z_l^O \) of closed and open HWs, respectively, on any 3D MSG fractal, scale with the number \( N_l = 4 N_G^{l} \) of the lattice sites as

\[
Z_l^C \sim \omega^{N_l} \left[ \lambda^{(N_G+k_c)/(N_G-3)} 4^{-\sigma} \right]^{N_{l}^{\sigma}}, \quad Z_l^O \sim \omega^{N_l} \left[ \lambda(k_c+3)/(N_G-3) 4^{-\sigma} \right]^{N_{l}^{\sigma}},
\]

doi:10.1088/1742-5468/2010/02/P02021 13
with \( \sigma \) given by formula (2.18):
\[
\sigma = \frac{\ln 3}{\ln(1/6)b(b+1)(b+2)} = \frac{\ln 3}{\ln b d_f}.
\]
Constants \( \omega \) and \( \lambda \) can be obtained numerically, using relations
\[
\ln \omega = \lim_{l \to \infty} \ln \frac{E_l}{N_l}, \quad \ln \lambda = \lim_{l \to \infty} \frac{\ln(B_l/E_l)}{3^l},
\]
and their particular values for \( b = 2, 3, \) and \( 4 \) are given in table 2. The number \( k_C = (b+1)(b+2)/2 - 8 \) represents the maximal number of \( G_l(b) \) generators within the \( G_{l+1}(b) \) that they belong to, which are traversed by a two-stranded \( E \)-type HW conformation (\( E \)-step) within any closed HW on \( G_{l+1}(b) \) (see equation (2.3) and appendix A). As one can see, HW conformations that traverse \( G_l(b) \), and recursion relations (2.5) for the corresponding numbers \( B_l \) and \( E_l \), are sufficient for obtaining the connectivity constant \( \omega \) that governs the leading exponential term in the scaling forms for \( Z_C \) and \( Z_O \), as well as the constant \( \lambda \) which appears in their correction terms. Whereas the leading term \( \omega N_l \) is the same for both closed and open HWs, the correction term has the same stretched exponential form \( \mu N_l^{\sigma} \) in the two cases, but with different values for \( \mu \) and \( \mu_O > \mu_C \), indicating that the number of open HWs is larger than the number of closed HWs. One should notice here that the fact that the scaling form obtained for open HWs is determined only by the behavior of the numbers \( B_l \) and \( E_l \) means that the contribution of one- and two-leg HW conformations (\( A, C, D \)- and \( H \)-type walks), i.e. HWs with their ends in the interior of \( G_l(b) \) fractal structures, is not significant. Furthermore, in sections 2 and 3 it was elaborated that the main mathematical reason for obtaining scaling forms with the stretched exponential correction term is the fact that \( \lim_{l \to \infty} B_l/E_l = 0 \), meaning that entangled conformations (with large numbers of two-stranded parts) dominate over those in which HWs rarely return to already visited fractal generators.

The results of the study of HWs on 3D MSG fractals presented in this paper should be compared with the results recently obtained for other fractal lattices [7]. For \( n \)-simplex fractal lattices with even values of \( n \) the same asymptotic behavior of the HW numbers was found, \( \omega N^{\mu N^\sigma} \), but with \( \sigma = 1/d_f \), which differs from the formula derived here for \( \sigma \). The existence of the term \( \mu N^\sigma \) was also related to the facts that: (1) entangled HWs prevail; and (2) HWs with ‘interior’ terminating points do not contribute to the asymptotic behavior of HW numbers, as in the 3D MSG fractals case. For odd \( n \), stretched exponential terms in the scaling forms for HWs on \( n \)-simplex fractals do not exist, HWs with ‘interior’ terminating points affect the scaling forms for the numbers of open HWs, and entangled conformations do not dominate in this case. For the Given–Mandelbrot and 2D modified Sierpinski gasket fractals (which are two-dimensional generalizations of the Sierpinski gasket and 3-simplex fractal, respectively), stretched exponential terms are also absent, whereas again, one- and two-leg conformations are necessary for obtaining the scaling forms for open HWs, and, due to the specific topology of these lattices, only one-stranded HW conformations are possible. Therefore, the results of the present study confirm the assumption that the existence of the stretched exponential term is related to the issue of HW entanglement. However, the discrepancy between the formulae obtained for the exponent \( \sigma \) for different fractal families and, more generally, the question of which properties of the underlying lattice determine \( \sigma \), and in what way, deserve further consideration. To this end we recall that stretched exponential terms were obtained for

\[\text{doi:10.1088/1742-5468/2010/02/P02021} \]
A model of compact polymers on a family of three-dimensional fractal lattices

HWs on Manhattan lattices [4] as well as low temperature SAWs on square [8]–[11] and cubic [12] lattices. In this context, one should also mention the spiral SAWs on 2D regular lattices [16] and lattice animals on some hierarchical lattices. Whereas, to the best of our knowledge, a physical interpretation of the stretched exponential term for the 2D spiral SAW models has never been proposed, its presence in the scaling forms obtained for lattice animals on hierarchical lattices was directly connected to the existence of the sets of sites with different coordination numbers [17]. Utilizing a similar idea, in the case of low temperature (collapsed) SAWs it was explicitly explained in [13] what the form

\[ \mu N_{\sigma} \]

with \( \sigma = (d - 1)/d \) for regular lattices, should arise. However, as was elaborated in [6,7], direct application of such an approach on HWs on fractal lattices does not give a satisfactory result. Yet, the scaling forms obtained in this paper can be expounded in the spirit of the physical reasoning given in [13], as will be explained in the following paragraph.

We shall first focus on closed HWs on \( G_l(b) \) with the maximal number of two-stranded \( E \)-type conformations within the unit tetrahedrons. Such HWs represent maximally entangled closed (MEC) compact conformations and they accomplish the maximal possible connectedness between the generators \( G_l(b) \) of all orders \( l \). Now, from all the \( N_l \) sites visited by such maximally entangled HWs, observe those which belong to one-stranded conformations (\( B \)-steps) within the unit tetrahedrons, and which are directly connected only to the sites belonging to the same unit tetrahedron. For instance, vertices 9 and 10, or 15 and 16 in figure 2 represent examples of such sites. Since these sites are not directly connected to the other tetrahedrons of the lattice (via HW), they are the maximally isolated sites within the maximally entangled closed HW conformation. It is shown in appendix E that the number \( N_{CI}^l \) of such sites is equal to

\[ N_{CI}^l = \frac{1}{2} N_G - k_C - 6 N_l + 2 \frac{N_G + k_C}{N_G - 3} 4^{-\sigma} N_l^\sigma, \] (4.1)

and one can easily see that, using this expression, the scaling relation for the numbers of closed HWs can be transformed into the following form:

\[ Z_l^C \sim \omega'^{N_l} \sqrt{\lambda}^{N_{CI}^l}, \] with \( \omega' = \omega/\lambda^{(N_G - k_C - 6)/(4(N_G - 3))} \). (4.2)

In a similar way (see appendix E), one can show that the scaling relation for open HWs can be expressed as

\[ Z_l^O \sim \omega'^{N_l} \sqrt{\lambda}^{N_{OI}^l}, \] (4.3)

where

\[ N_{OI}^l = \frac{1}{2} N_G - k_C - 6 N_l + 2 \frac{k_C + 3}{N_G - 3} 4^{-\sigma} N_l^\sigma \] (4.4)

is the number of maximally isolated sites on \( G_l(b) \) visited by a maximally entangled open HW (which is an open HW with the maximal number of \( E \)-steps on unit tetrahedrons and with both loose ends being of type \( C \), on all levels \( l \)). Comparing forms (4.2) and (4.3) with the scaling relations expected for HWs on homogeneous lattices, one can say that in this case terms \( \sqrt{\lambda}^{N_{CI}^l} \) and \( \sqrt{\lambda}^{N_{OI}^l} \) play the role of the stretched exponential correction term \( \mu N_{\sigma}^l \) in the case of homogeneous lattices. Indeed, for homogeneous lattices, \( N_{\sigma}^l \), with \( \sigma = (d - 1)/d \), is proportional to the number of sites on the lattice boundary which have

doi:10.1088/1742-5468/2010/02/P02021
smaller number of neighbors than the bulk sites, and in that sense they are similar to the maximally isolated sites within the maximally entangled HWs on 3D MSG lattices. Therefore, one might generally expect the scaling relation for the number of HWs on nonhomogeneous lattices to have, instead of the stretched exponential correction term, a term $\mu N$, where $N_I$ is the number of conveniently defined ‘maximally isolated sites’. The relation between $N_I$ and the overall number of lattice sites $N$ depends on the particular topology of the lattice under study, which is why different scaling forms, as functions of $N$, are obtained.

The conclusion of the previous paragraph can be supported by performing a similar analysis in the case of HWs on previously studied fractal families [7]. For instance, for $n$-simplex fractals, maximally isolated sites can be defined like for 3D MSG fractals, i.e. these are the sites which are directly connected by maximally entangled HWs only with the sites within the same fractal generator as they belong to. Here, maximally entangled HWs are those that contain the maximal number of maximally stranded HW parts. Then, it can be shown [18] that $N_{CI}^O = (n/2)N^O$ and $N_{CI}^C = ((n/2) - 1)N^C$, where $\sigma = \ln 2/\ln n$. Since overall numbers of closed and open HWs on the $n$-simplex fractal with even $n$ asymptotically behave as $Z_C^O \sim \omega N^O \lambda_B^{N^O}$ (formula (5.8) in [7]) and $Z_C^O \sim \omega N^O \lambda_B^{(n-2)/2}N^P$, where $\omega' = \omega$ and $\mu = \lambda_B$ for both kinds of HWs. For odd values of $n$, however, it can be shown [18] that the number $N_I$ of maximally isolated sites, for both open and closed HWs, is proportional to $N_I$, so any term of the form $\mu N_I$ can only contribute to the leading term $\omega N$. This certainly is in accord with the scaling forms found in [7] for odd $n$, which do not have stretched exponential corrections.

To conclude, we may say that the exact study of Hamiltonian walks on modified three-dimensional Sierpinski gasket fractals presented supports the idea that entangled conformations are of the most physical importance for the behavior of compact polymers in inhomogeneous media. The concept of ‘maximally isolated sites’ introduced proved to be useful in the physical interpretation of different scaling forms obtained for Hamiltonian walks on all fractals studied so far. Whether such a concept can be applied to homogeneous and other nonhomogeneous lattices will be a subject of our further investigations.

Acknowledgment

This paper was produced within Project No. OI 141020B, funded by the Serbian Ministry of Science and Environmental Protection.

Appendix A. The maximal number of $E$-steps within HW configurations

In this appendix we prove that the numbers $k_C$, $k_B$ and $k_E$ are given by formulae (2.4) and (2.7). The number $k_C$ is the maximum number of $E$-steps within the closed HW configuration (see (2.3)), whereas the numbers $k_B$ and $k_E$ are related to the maximum number of $E$-steps within the HW configurations of $B$ and $E$ type (see (2.5)), i.e. the conformations that traverse the generator of order $l + 1$ once or twice, respectively. By an ‘$E$-step’ here we imply any HW conformation consisting of two mutually avoiding strands, both traversing the generator of order $l$ (see figure 2). In a similar way, a ‘$B$-step’ is any HW conformation that consists of one strand traversing $G_l(b)$.
A model of compact polymers on a family of three-dimensional fractal lattices

Figure A.1. On the left-hand side of this picture generator $G_{l+1}(b)$ of order $l+1$, for $b = 4$ 3D MSG, is presented, as seen from above. Gray-shaded small tetrahedrons represent generators $G_l(4)$ of order $l$, lower layers being darker. Vertices lying in the same horizontal plane are indicated with the same symbol, also being the same for two adjacent planes containing vertices that belong to different generators. On the right-hand side of the picture horizontal layers of tetrahedrons are split and slightly magnified in order that all vertices, as well as some junctions, can be seen. In particular, twofold junctions in the lowest layer of vertices are indicated by yellow lines, whereas junctions joining three vertices are given in green. There is only one fourfold junction—the corresponding four connected vertices are encircled, and in the magnified circle these vertices are presented as seen in three dimensions, with the junction indicated in orange. One can check that the overall number of junctions is $N_J = 31$ (three twofold junctions for each of six $G_{l+1}(4)$ edges, three threefold junctions for each of four $G_{l+1}(4)$ faces, and one fourfold interior junction), which certainly is in accord with formula (A.1).

According to our definition of the modified Sierpinski gasket fractals, generators $G_l(b)$ within the generator $G_{l+1}(b)$ are connected via infinitesimal junctions. Each of these junctions connects two, three or four neighboring $G_l(b)$ generators. A ‘twofold’ junction connects vertices of neighboring generators $G_l(b)$, both lying in the same edge of $G_{l+1}(b)$ (for instance, vertices 3 and 4 in figure 2 are joined by such a junction). Vertices of neighboring generators $G_l(b)$ that lie inside the faces of $G_{l+1}(b)$ (such as sites 5, 6 and 19 in figure 2) are connected by threefold junctions, whereas fourfold junctions occur in the interior of $G_{l+1}(b)$, and can exist only for $b \geq 4$. In figure A.1 we explicitly indicate some of the junctions connecting the vertices of the generators $G_l(4)$, within the generator $G_{l+1}(4)$. It is not difficult to show that the number of junctions which connect $N_G$ generators $G_l(b)$ to the generator $G_{l+1}(b)$ is equal to

$$N_J = \frac{1}{6}(b + 1)(b + 2)(b + 3) - 4. \quad (A.1)$$

doi:10.1088/1742-5468/2010/02/P02021
From the constraint that each site of the lattice has to be visited exactly once, it follows that each junction (i.e. its middle point) can be traversed at most once. Now, suppose that a closed HW conformation within $G_{i+1}(b)$ consists of $\alpha$ $B$-steps and $\beta$ $E$-steps. Each $G_i(b)$ is traversed by the HW, which implies that

$$\alpha + \beta = N_G = \frac{1}{6} b(b+1)(b+2). \quad (A.2)$$

Each $B$-step uses two junctions and each $E$-step uses four junctions. However, since each junction connects two $G_i(b)$ generators, the overall number of junctions visited is equal to $\alpha + 2\beta$. In addition, steps through corner $G_i(b)$ generators for the closed HW have to be of $B$ type (see figure 2), which means that one of the three junctions for each of the four corner generators is certainly not used. This implies that the inequality

$$\alpha + 2\beta \leq N_J - 4 = \frac{1}{6} b(b+1)(b+2)(b+3) - 8 \quad (A.3)$$

is satisfied. Then, from (A.2) and (A.3) it directly follows that

$$\beta \leq \frac{1}{3} (b+1)(b+2) - 8, \quad (A.4)$$

i.e. the maximum number of $E$-steps within the closed HW conformation is indeed equal to

$$\beta_{\text{max}} = k_C = \frac{1}{3} (b+1)(b+2) - 8. \quad (A.5)$$

Next, we consider a $B$-type HW configuration on a $G_{i+1}(b)$ generator, with $\alpha$ $B$-steps and $\beta$ $E$-steps. Steps through two corner $G_i(b)$ generators, at which HW starts or terminates, can be of either $B$ or $E$ type. However, both of the remaining two corner $G_i(b)$ generators must be traversed by a $B$-step (see figure A.2), meaning that two of the $N_J$ junctions are never used. On the other hand, each $B$-step uses two junctions, unless it is the first or the last step of the HW configuration, in which case it utilizes only one junction (since the corner vertex does not belong to any junction). Similarly, an $E$-step which traverses the interior $G_i(b)$ generators uses four junctions, whereas a possible $E$-step through either the first or the last traversed $G_i(b)$ uses only three junctions. Suppose that both the first and the last visited corner generators contain an $E$-step. Then, these two steps together use six junctions, and the remaining $(\beta - 2)$ ‘interior’ $E$-steps use $4(\beta - 2)$, whereas $\alpha$ $B$-steps use $2\alpha$ junctions. Since every junction can be traversed only once, and two consecutive steps share junctions, it follows that altogether $[6 + 4(\beta - 2) + 2\alpha]/2$ junctions are visited by such HW conformations. This implies the following inequality:

$$\frac{1}{2} [6 + 4(\beta - 2) + 2\alpha] \leq N_J - 2, \quad (A.6)$$

which, together with the relation $\alpha + \beta = N_G$, gives

$$\beta \leq N_J - N_G - 1 = \frac{1}{3} (b+1)(b+2) - 5 = \beta_{\text{max}} = N_G - k_B. \quad (A.7)$$

In the remaining two possible situations, when either the first and the last $G_i(b)$ are traversed by $B$-steps, or one of them is traversed by a $B$-step and the other by an $E$-step, it can be shown in a similar way that inequality (A.7) holds as well.

As one can see in figure A.3 an $E$-type HW conformation within $G_{i+1}(b)$ can use all three junctions of any corner $G_i(b)$, which happens when such a $G_i(b)$ is traversed by an $E$-step. This also means that all $N_J$ junctions within $G_{i+1}(b)$ can be utilized. Suppose that all four corner $G_i(b)$ generators are traversed by $E$-steps—altogether 12 junctions
A model of compact polymers on a family of three-dimensional fractal lattices

Figure A.2. Generator $G_{l+1}(5)$, viewed from above, with the upper three layers of constitutive generators $G_l(5)$ (gray-shaded tetrahedrons/triangles) moved to the right-hand side of the picture, for the sake of better visualization. The red oriented line represents a $B$-type HW configuration, which contains 16 $E$-steps, i.e. the maximum possible number of them, given by formula (A.7). The remaining 19 steps are of the $B$ type, and they are depicted as straight lines connecting only two vertices of the traversed $G_l(5)$ generator, but it is implied that all sites within it are visited. The numbers in the figure denote points where the HW leaves or enters the lower part of $G_{l+1}(5)$.

are used by these four $E$-steps. If the whole HW conformation contains $\beta$ $E$-steps, the remaining $(\beta - 4)$ interior $E$-steps take $4(\beta - 4)$ junctions, whereas to all $\alpha$ $B$-steps, $2\alpha$ junctions correspond. Every junction used connects two steps; therefore in this case the inequality

$$\frac{1}{2}[12 + 4(\beta - 4) + 2\alpha] \leq N_J,$$

(A.8)

holds, which, again with $\alpha + \beta = N_G$, leads to

$$\beta \leq N_J - N_G + 2 = \beta_{\text{max}} = \frac{1}{2}(b+1)(b+2) - 2 = N_G - k_E.$$ (A.9)

In a similar manner one can show that in the remaining four possibilities: one, two, three or four $B$-steps through the corner $G_l(b)$ generators, inequality (A.9) is valid again.

Note that formulae (A.5), (A.7) and (A.9) are not correct in the $b = 2$ case. In this case all four constitutive $G_l(b = 2)$ generators of the $G_{l+1}(b = 2)$ generator are at its corners, and each of them is connected to each of the other three by a twofold junction. Since two corner generators have a junction in common, the numbers of usable junctions in relations (A.3) and (A.6) are $N_J - 2$ and $N_J - 1$ instead of $N_J - 4$ and $N_J - 2$, respectively. If we represent each $G_l(2)$ by a point (vertex), then $G_{l+1}(2)$ represents a complete graph of four points. Since there can be neither a subgraph with three points of degree 3 and one point of degree 1 nor a subgraph with two points of degree 3 and two of degree 1, terms in relation (2.6) with $E^3$ and $E^2$ are not possible.
Appendix B. Asymptotical behavior of the parameter $x_l = B_l/E_l$

As was stressed in section 2, the asymptotical behavior of the parameter $x_l = B_l/E_l$ is of the greatest importance for obtaining the scaling form of HWs. Here we want to prove that the assumption that $p_{kE+k} > m_{kE+k+1}$, for $2 \leq k \leq k_C + 5$, leads to the conclusion that $x_l \to 0$, when $l \to \infty$. The numbers $x_l$ satisfy the exact relation (2.8), from which it follows that

$$x_{l+1} - x_l = x_l \frac{-p_{kE} - p_{kE+1} x_l - p_{kE+kC+6} x_l^{kC+6} - \sum_{k=2}^{kC+5} (p_{kE+k} - m_{kE+k+1}) x_l^k}{\sum_{k=0}^{kC+6} p_{kE+k} x_l^k} < 0,$$

where we used the relation $k_E = k_B - 3$, obtained in the previous appendix, and the fact that all coefficients $p_k$ and $m_k$ are positive, as well as the proposed inequality. This means that the sequence of positive numbers $x_l$ is monotonically decreasing, and since $x_0 = 2$, it follows that this sequence has non-negative limiting value $c = \lim_{l \to \infty} x_l$. If $c > 0$, again from (2.8), when $l \to \infty$, the equation

$$c = c^3 \frac{\sum_{k=0}^{kC+3} m_{kE+k} c^k}{\sum_{k=0}^{kC+6} p_{kE+k} c^k}$$

follows which, after dividing by $c$, can be transformed to

$$0 = p_{kE} + p_{kE+1} c + p_{kE+kC+6} c^{kC+6} + \sum_{k=2}^{kC+5} (p_{kE+k} - m_{kE+k+1}) c^k.$$

However, the latter equation cannot be satisfied, since its right-hand side has the form of a polynomial in $c$, with all its coefficients being positive numbers. Consequently, one concludes that $c = 0$.

doi:10.1088/1742-5468/2010/02/P02021
generators are traversed by respectively using one, three, or two junctions. Two of the remaining three corner steps can be either of (3.8). It is obvious that the dangling end-step of a one-leg configuration within its corresponding three junctions can be traversed. Now, suppose that the corner steps contain an A-traversed by a

\[ \alpha + 2\beta = N_G - 1 \]  

is satisfied.

Consider an A-type HW configuration on generator \( G_{l+1}(b) \). One of its end-steps is fixed at one of the four corner generators \( G_l(b) \) and it can be a B-, E-, or C-step, respectively using one, three, or two junctions. Two of the remaining three corner generators are traversed by B-steps, each of them using two junctions of the corresponding \( G_l(b) \), whereas its third junction cannot be traversed. The last corner generator is either traversed by a B-step or contains a dangling A- or C-step, and such steps use two, one, or three junctions, respectively. If a corner generator contains an A-step, only one of its corresponding three junctions can be traversed. Now, suppose that the ‘corner’ steps are \( EBBB \), whereas the dangling A-step, using one junction, is in the interior generator. Such an HW traverses \( (3 + 2\alpha + 4(\beta - 1) + 1)/2 = \alpha + 2\beta \) junctions, and, since corner B-steps cannot use altogether three of all the \( N_J \) junctions, it follows that

\[ \alpha + 2\beta \leq N_J - 3, \]  

\[ \beta_{\max} \]  

| Dangling end-step and its position | ‘Corner’ passing steps | ‘Corner’ fixed step | Number of junctions used | Number of usable junctions | \( \beta_{\max} \) |
|-----------------------------------|-----------------------|-------------------|-------------------------|--------------------------|---------------------|
| A—interior \( G_l(b) \)           | BBB                   | E                 | \( \alpha + 2\beta \)   | \( N_J - 3 \)             | \( N_J - N_G - 2 \) |
| A—interior \( G_l(b) \)           | BBB                   | B                 | \( \alpha + 2\beta \)   | \( N_J - 5 \)             | \( N_J - N_G - 4 \) |
| A—corner \( G_l(b) \)             | BB                    | E                 | \( \alpha + 2\beta \)   | \( N_J - 4 \)             | \( N_J - N_G - 3 \) |
| A—corner \( G_l(b) \)             | BB                    | B                 | \( \alpha + 2\beta \)   | \( N_J - 6 \)             | \( N_J - N_G - 5 \) |
| C—interior \( G_l(b) \)           | BBB                   | E                 | \( 1 + \alpha + 2\beta \) | \( N_J - 3 \)             | \( N_J - N_G - 2 \) |
| C—interior \( G_l(b) \)           | BBB                   | B                 | \( 1 + \alpha + 2\beta \) | \( N_J - 5 \)             | \( N_J - N_G - 5 \) |
| C—corner \( G_l(b) \)             | BB                    | E                 | \( 1 + \alpha + 2\beta \) | \( N_J - 2 \)             | \( N_J - N_G - 2 \) |
| C—corner \( G_l(b) \)             | BB                    | B                 | \( 1 + \alpha + 2\beta \) | \( N_J - 4 \)             | \( N_J - N_G - 4 \) |
| C—corner \( G_l(b) \)             | BBB                   | C                 | \( 1 + \alpha + 2\beta \) | \( N_J - 4 \)             | \( N_J - N_G - 4 \) |

In this appendix we first show that polynomials \( R_{ij} \) appearing in recursion relations (3.2) for numbers \( A_l \) and \( C_l \) of one-leg HW conformations have the form (3.3), with \( k_{ij} \) given by (3.8). It is obvious that the dangling end-step of a one-leg configuration within \( G_{l+1}(b) \) can be either of \( A \) type or of \( C \) type. The remaining part of the HW traverses the remaining \( N_G - 1 \) generators \( G_l(b) \), and consists of \( \alpha \) B-steps and \( \beta \) E-steps, so the equation

\[ \alpha + \beta = N_G - 1 \]  

(\( \beta_{\max} \))

\[ \beta_{\max} \]  

Appendix C. Recursion relations for the numbers \( A_l \), \( C_l \) and \( Z_l^O \)

A model of compact polymers on a family of three-dimensional fractal lattices

Table C.1. All possible situations for an \( A \)-type HW configuration on \( G_{l+1}(b) \), depending on the type of its dangling end-step, steps traversing corner generators \( G_l(b) \) and the end-step fixed in one of the corners. For each situation the corresponding numbers of passed and usable junctions, as well as the maximum possible value of the number \( \beta \) of E-steps, are given.

\[ \alpha + 2\beta + 1 \leq N_J - 3 \]  

(3.2)

\[ \beta_{\max} \]  

\[ \beta_{\max} \]  

\[ \beta_{\max} \]  

\[ \beta_{\max} \]  

doi:10.1088/1742-5468/2010/02/P02021
A model of compact polymers on a family of three-dimensional fractal lattices

Table C.2. Description of possible C-type HW configurations on $G_{l+1}(b)$, depending on the type of the dangling end-step, and the steps within corner generators $G_l(b)$. For each situation the corresponding numbers of passed and usable junctions, as well as the maximum possible value of the number $\beta$ of $E$-steps, are given.

| Dangling end-step and its position | ‘Corner’ fixed steps | ‘Corner’ passing step | Number of junctions used | Number of usable junctions | $\beta_{\text{max}}$ |
|-----------------------------------|---------------------|----------------------|--------------------------|---------------------------|----------------------|
| $A$—interior $G_l(b)$             | BBB                 | B                    | $\alpha + 2\beta - 1$   | $N_j - 7$                 | $N_j - N_G - 5$      |
| $A$—interior $G_l(b)$             | BBE                 | B                    | $\alpha + 2\beta - 1$   | $N_j - 5$                 | $N_j - N_G - 3$      |
| $A$—corner $G_l(b)$              | BEE                 | B                    | $\alpha + 2\beta - 1$   | $N_j - 3$                 | $N_j - N_G - 1$      |
| $A$—corner $G_l(b)$              | EEE                 | B                    | $\alpha + 2\beta - 1$   | $N_j - 1$                 | $N_j - N_G + 1$     |
| $A$—corner $G_l(b)$              | BBB                 | A                    | $\alpha + 2\beta - 1$   | $N_j - 8$                 | $N_j - N_G - 6$      |
| $A$—corner $G_l(b)$              | BBE                 | A                    | $\alpha + 2\beta - 1$   | $N_j - 6$                 | $N_j - N_G - 4$      |
| $A$—corner $G_l(b)$              | BEE                 | A                    | $\alpha + 2\beta - 1$   | $N_j - 4$                 | $N_j - N_G - 2$      |
| $A$—corner $G_l(b)$              | EEE                 | A                    | $\alpha + 2\beta - 1$   | $N_j - 2$                 | $N_j - N_G$          |
| $C$—interior $G_l(b)$            | BBB                 | B                    | $\alpha + 2\beta$       | $N_j - 7$                 | $N_j - N_G - 6$      |
| $C$—interior $G_l(b)$            | BBE                 | B                    | $\alpha + 2\beta$       | $N_j - 5$                 | $N_j - N_G - 4$      |
| $C$—interior $G_l(b)$            | BEE                 | B                    | $\alpha + 2\beta$       | $N_j - 3$                 | $N_j - N_G - 2$      |
| $C$—corner $G_l(b)$              | EEE                 | B                    | $\alpha + 2\beta$       | $N_j - 1$                 | $N_j - N_G$          |
| $C$—corner $G_l(b)$              | BBE                 | C                    | $\alpha + 2\beta$       | $N_j - 6$                 | $N_j - N_G - 5$      |
| $C$—corner $G_l(b)$              | BEE                 | C                    | $\alpha + 2\beta$       | $N_j - 4$                 | $N_j - N_G - 3$      |
| $C$—corner $G_l(b)$              | EEE                 | C                    | $\alpha + 2\beta$       | $N_j - 2$                 | $N_j - N_G + 1$     |

which with (C.1) gives

$$\beta \leq N_j - N_G - 2 = \frac{1}{2}(b + 1)(b + 2) - 6 = k_C + 2.$$  \hfill (C.3)

In a similar manner one can analyze all the other possibilities and obtain the corresponding maximum value of $\beta$. From table C.1, in which all of these possibilities, together with the corresponding numbers of junctions that are used and usable, as well as $\beta_{\text{max}}$, are given, one can see that $k_{11} = k_{12} = k_C + 2$.

A $C$-type HW configuration on $G_{l+1}(b)$ consists of two strands: one of $B$ type, i.e. with two ends fixed at two corners of the $G_{l+1}(b)$, and the other of $A$ type, with one end fixed at the third corner, whereas its second end is free, i.e. it can be anywhere within the $G_{l+1}(b)$, in some of the interior generators $G_l(b)$, as well as in any of the four corner generators $G_l(b)$. The three steps containing fixed ends can be of either $B$ or $E$ type, whereas the corner generator, which does not contain the fixed end, is either traversed by a $B$-step or contains the dangling $A$- or $C$-step. The other relevant details of possible situations, regarding the type and the position of the step containing the dangling end, are listed in table C.2. One can see that HW configurations with $A$ dangling end-step and maximal number of $E$-steps are those with the dangling end-step in the interior $G_l(b)$, whereas the three steps with ends fixed at corner generators are of $E$ type, and the fourth corner...
In the remaining part of this appendix we show that polynomials \( F \) and \( S \) appearing in the recursion relation (3.1) for the overall number \( Z_{l+1}^{(G)} \) of open HWs on \( G_{l+1}(b) \) have the form given by (3.5). Polynomials \( F_{AA}, F_{AC} \) and \( F_{CC} \) correspond to HWs whose two end-steps are two \( A \)-steps, one \( A \)-step and one \( C \)-step, and two \( C \)-steps, respectively. Since the whole HW configuration has \( N_G \) steps, its ‘interior’ part has \( N_G - 2 \) steps which are either of \( B \) or \( E \) type, implying that \( F_{XY} \) are homogeneous polynomials in \( B_l \) and \( E_l \) of power \( N_G - 2 \). In table C.3 we list all possible arrangements of steps within open HW configuration with two one-leg end-steps, together with the corresponding numbers of junctions that are used and usable. Using these data one can recognize arrangements with the maximum possible number of \( E \)-steps, and conclude that this number is equal to \( N_1 - N_G - 3 = k_C + 1 \).

If an open HW has both of its ends in the same \( G_l(b) \), then this corresponds to a \( D \)- or \( H \)-step within it, whereas the remaining part of that HW consists of \( \alpha \) \( B \)-steps and \( \beta \) \( E \)-steps such that \( \alpha + \beta = N_G - 1 \). This means that \( S_{D} \) and \( S_{H} \) are homogeneous polynomials in \( B_l \) and \( E_l \) of power \( N_G - 1 \). An \( H \)-step can exist only in the interior \( G_l(b) \), in which case all steps through corner generators are of \( B \) type, and four junctions can never be utilized. Since such an HW takes \( 2 + \alpha + 2\beta \) junctions, it follows that \( \beta \leq N_1 - N_G - 5 = k_C - 1 \). Finally, a \( D \)-step can exist in any \( G_l(b) \), either a corner or an interior one, but in both cases the number of junctions used is \( 1 + \alpha + 2\beta \), and four junctions corresponding to corner generators cannot be taken by such an HW. Thus, one obtains that the maximum number of \( E \)-steps is \( \beta_{\text{max}} = N_1 - N_G - 4 = k_C \).
Appendix D. Two-leg HW configurations

Here we give some details of the derivation of the conclusion that the numbers of two-leg HW configurations are not needed for obtaining the scaling form of the overall number of open HWs.

First we notice that the recursion relation for the two-leg HW configuration of the type $D$, given in (3.4), follows from the fact that dangling ends of the two strands can reside either (1) in the same generator $G_i(b)$, thus forming a $D$- or $H$-step within it, or (2) in two different generators $G_i(b)$, thus forming two one-leg steps, either of $A$ or $C$ type. It is not difficult to see that case (1) can be obtained by cutting a step of some $B$-type configuration. Therefore, each $B$-type configuration with $(N_G-k)$ $E$-steps gives rise to $k$ $D$-type configurations with $(N_G-k)$ $E$-steps and one $D$-step, which are obtained by cutting a $B$-step, whereas by cutting its $E$-steps (which can be done in two ways for each $E$-step) one can obtain $2(N_G-k)$ different $D$-type configurations with $k$ $B$-steps, $(N_G-k-1)$ $E$-steps and one $H$-step. In a similar way, by cutting an $E$-type HW configuration, one can obtain an $H$-type configuration. From these observations it straightforwardly follows that

$$d_D(B,E) = \sum_{k=k_E}^{N_G} km_k B^{k-1} E^{N_G-k}, \quad d_H(B,E) = 2 \sum_{k=k_E}^{N_G} (N_G-k) m_k B^k E^{N_G-k-1},$$

$$h_D(B,E) = \frac{1}{2} \sum_{k=k_E}^{N_G} k p_k B^{k-1} E^{N_G-k}, \quad h_H(B,E) = \sum_{k=k_E}^{N_G} (N_G-k) p_k B^k E^{N_G-k-1}. \tag{D.1}$$

Applying a reasoning similar to that used in the previous appendix, one can obtain that polynomials $d_{XY}$ and $h_{XY}$, corresponding to two-leg configurations with dangling ends in different generators, have the following forms:

$$d_{XY}(B,E) = \sum_{k=0}^{k_{XY}+4} s_k^{XY} B^{N_G-2-k} E^k, \quad h_{XY}(B,E) = \sum_{k=0}^{k_{XY}} o_k^{XY} B^{N_G-2-k} E^k, \tag{D.2}$$

with $s_k^{XY}$ and $o_k^{XY}$ being constant positive integers, $XY = AA, AC, CC$, and

$$k_{AA} = k_C + 7 = k_{AC} + 1 = k_{CC} + 2.$$

Next, the recursion relations (3.10) are obtained by dividing (3.4) by the recursion relation for $E_i$, given in (2.5). Therefore, coefficients $p_{ij}$ are defined as

$$p_{11}(x_i) = \frac{d_D(B_i, E_i) E_i}{E_{i+1}(B_i, E_i)}, \quad p_{12}(x_i) = \frac{d_H(B_i, E_i) E_i}{E_{i+1}(B_i, E_i)},$$

$$p_{21}(x_i) = \frac{h_D(B_i, E_i) E_i}{E_{i+1}(B_i, E_i)}, \quad p_{22}(x_i) = \frac{h_H(B_i, E_i) E_i}{E_{i+1}(B_i, E_i)},$$

and $t_{ji}$ as

$$t_{11}(x_i) = \frac{d_{XY}(B_i, E_i) E_i^2}{E_{i+1}(B_i, E_i)}, \quad t_{21}(x_i) = \frac{h_{XY}(B_i, E_i) E_i^2}{E_{i+1}(B_i, E_i)},$$

where $i = 1, 2, 3$ corresponds to $XY = AA, AC, CC$, respectively. Then, from (D.1) and (D.2) relations (3.11) directly follow.
For \( l \gg 1 \), \( x_l \) tends to 0, so from (3.11) one obtains
\[
\begin{align*}
p_{11}(x_l) &\approx k_B \frac{mk_B}{p_{kB}} x_l^2, & p_{12}(x_l) &\approx 2(k_C + 3) \frac{mk_B}{p_{kB}} x_l^3, & p_{21}(x_l) &\approx k_E \frac{1}{2} \frac{1}{x_l}, \\
p_{22}(x_l) &\approx k_C + 6, & t_{11}(x_l) &\approx \frac{s_{kC+4}^{XY}}{p_{kE}}, & t_{21}(x_l) &\approx \frac{o_{kC+7}^{AA}}{p_{kE}} \frac{1}{x_l^3}, \\
t_{22}(x_l) &\approx \frac{o_{kC+6}^{AC}}{p_{kE}} \frac{1}{x_l}. & t_{23}(x_l) &\approx \frac{o_{kC+5}^{CC}}{p_{kE}} \frac{1}{x_l}.
\end{align*}
\]

Finally, using these approximate forms while multiplying (3.10) with (2.9), relation (3.12) is obtained, with coefficients \( a_{ij} \) equal to
\[
\begin{align*}
a_{11} &= k_B \left( \frac{mk_B}{p_{kB}} \right)^3, & a_{12} &= 2(k_C + 3) \left( \frac{mk_B}{p_{kB}} \right)^3, \\
a_{21} &= \frac{k_E}{2} \left( \frac{mk_B}{p_{kB}} \right)^3, & a_{22} &= (k_C + 6) \left( \frac{mk_B}{p_{kB}} \right)^3,
\end{align*}
\]
and
\[
b_{13} = \frac{s_{kC+4}^{CC}}{p_{kE}} \left( \frac{mk_B}{p_{kB}} \right)^2.
\]

**Appendix E. Maximally isolated sites within maximally entangled HWs**

In this appendix we want to derive the formulae (4.1) and (4.4) for the numbers \( N^C_{l} \) and \( N^O_{l} \) of maximally isolated sites within the maximally entangled closed (MEC) and maximally entangled open (MEO) Hamiltonian walks, respectively. Since MEC HWs on the generator \( G_l(b) \) of order \( l \) are closed HWs with the maximal number of \( E \)-steps, and maximally isolated sites within MEC HW are ‘interior’ vertices of \( B \)-steps made through unit tetrahedrons (i.e. not the vertices at which the HW enters or exits the tetrahedron), the number \( N^C_{l} \) is equal to
\[
N^C_{l} = 2N^B_{l},
\]
where \( N^B_{l} \) is the number of unit tetrahedrons traversed by \( B \)-steps. In order to calculate \( N^B_{l} \), and consequently \( N^C_{l} \), we observe maximally entangled \( B \)-type (MEB) HWs, i.e. \( B \)-type HWs with the maximal number of \( E \)-steps, and, similarly, maximally entangled \( E \)-type (MEE) HWs. For the MEB HW passing through the \( G_{l+1}(b) \) generator, we introduce the label \( N^B_{l+1} \) for the numbers of unit tetrahedrons traversed by a \( B \)-step. In a similar way, let \( N^E_{l+1} \) be the number of unit tetrahedrons of \( G_{l+1}(b) \) traversed by a \( B \)-step for an MEE HW. Then, from the recursion relation for the numbers \( B_l \) and \( E_l \) (2.5) there follows the matrix recursion relation for the numbers \( N^B_{l} \) and \( N^E_{l} \):
\[
\begin{pmatrix}
N^B_{l+1} \\
N^E_{l+1}
\end{pmatrix} =
\begin{pmatrix}
k_B & N_G - k_B \\
k_E & N_G - k_E
\end{pmatrix}
\begin{pmatrix}
N^B_{l} \\
N^E_{l}
\end{pmatrix}.
\]

\[\text{doi:10.1088/1742-5468/2010/02/P02021}\]
Since $k_B$ and $k_E$ are given by (2.7), and for the unit tetrahedron one has $N_{0}^{BB} = 1$ and $N_{0}^{EB} = 0$, solving the recursion relation obtained one obtains

$$N_{l}^{BB} = \frac{3 + k_{C} 3^{l}}{N_{G} - 3} + \frac{N_{G} - k_{C} - 6}{N_{G} - 3} N_{l}^{G},$$

(E.3)

$$N_{l}^{EB} = -\frac{N_{G} - k_{C} - 6}{N_{G} - 3} 3^{l} + \frac{N_{G} - k_{C} - 6}{N_{G} - 3} N_{l}^{G}.$$  

(E.4)

Taking into account that the MEC HW on $G_{l+1}(b)$ consists of $k_{C}$ MEE HWs on $G_{l}(b)$ generators and $(N_{G} - k_{C})$ MEB HWs on $G_{l}(b)$, as implied by (2.3), it follows that

$$N_{l+1}^{B} = (N_{G} - k_{C})N_{l}^{BB} + k_{C}N_{l}^{EB},$$

and consequently

$$N_{l}^{B} = \frac{N_{G} + k_{C} 3^{l}}{N_{G} - 3} + \frac{N_{G} - k_{C} - 6}{N_{G} - 3} N_{l}^{G}.$$  

(E.5)

Since $N_{l}^{CI} = 2N_{l}^{B}$, $N_{l} = 4N_{l}^{B}$, and $\sigma = \ln 3/\ln N_{G}$, as given by (2.18), formula (4.1) follows straightforwardly. In a similar manner, from (3.1), (3.2), (3.3), (3.5), (3.8), and (E.4) for the MEO case, one obtains (4.4).

References

[1] Vanderzande C, 1998 Lattice Models of Polymers (Cambridge: Cambridge University Press)

[2] Flory P J, 1956 Proc. R. Soc. A 234 60

[3] Dill K A, 1999 Protein Sci. 8 1166

[4] Duplantier B and David F, 1988 J. Stat. Phys. 51 327

[5] Bradley R M, 1989 J. Phys. A: Math. Gen. 22 L19

[6] Stajić J and Elezović-Hadžić S, 2005 J. Phys. A: Math. Gen. 38 5677

[7] Elezović-Hadžić S, Marčetić D and Maletić S, 2007 Phys. Rev. E 76 011107

[8] Prellberg T, Owczarek A L, Brak R and Guttmann A J, 1993 Phys. Rev. E 48 2386

[9] Owczarek A L, 1993 J. Phys. A: Math. Gen. 26 L647

[10] Bennet-Wood D, Brak R, Guttmann A J, Owczarek A L and Prellberg T, 1994 J. Phys. A: Math. Gen. 27 L1

[11] Ballesteros M, Orlandini E and Stella A L, 2006 Phys. Rev. Lett. 96 040602

[12] Grassberger P and Hegger R, 1995 J. Chem. Phys. 102 6881

[13] Owczarek A L, Prellberg T and Brak R, 1993 Phys. Rev. Lett. 70 951

[14] Mayer J-M, Guez C and Dayantis J, 1990 Phys. Rev. B 42 660

[15] Ramakrishnan R, Pekny J F and Caruthers J M, 1995 J. Chem. Phys. 103 7592

[16] Jaeckel A, Sturm J and Dayantis J, 1997 J. Phys. A: Math. Gen. 30 2345

[17] Lua R, Borovinskiy A L and Grosberg A Yu, 2004 Polymer 45 717

[18] Mansfield M L, 2006 J. Chem. Phys. 125 154103

[19] Oberdorf R, Ferguson A, Jacobsen J L and Kondev J, 2006 Phys. Rev. E 74 051801

[20] Jacobsen J L, 2008 Phys. Rev. Lett. 100 118102

doi:10.1088/1742-5468/2010/02/P02021
A model of compact polymers on a family of three-dimensional fractal lattices

[16] Blöte H W J and Hilhorst H J, 1984 J. Phys. A: Math. Gen. 17 L111
    Guttmann A J and Wormald N C, 1984 J. Phys. A: Math. Gen. 17 L271
    Guttmann A J and Wallace K J, 1986 J. Phys. A: Math. Gen. 19 1645

[17] Knežević D, Djordjević K and Knežević M, 2007 J. Stat. Mech. P12007

[18] Lekić D, 2009 Private communication