Effects of the boundaries on the scaling form of Hamiltonian walks on fractal lattices

D Marčetić1, S Elezović-Hadžić2 and I Živić3

1Faculty of Natural Sciences and Mathematics, University of Banja Luka, M. Stojanovića 2, 78000 Banja Luka, Bosnia and Herzegovina
2Faculty of Physics, University of Belgrade, P.O. Box 44, 11001 Belgrade, Serbia
3Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia

E-mail: dusanka.marcetic-lekic@pmf.unibl.org

Abstract. Hamiltonian walks (HWs) on a lattice are random walks that visit each lattice site exactly once. They are commonly used to model compact polymer conformations. The scaling form for the number of HWs, on translationary invariant lattices, consists of the leading exponential factor with the power law and stretched exponential factor as corrections. The stretched exponential factor, with the exponent $\sigma$ that depends on the lattice dimension only, is caused and determined by the boundary sites of the lattice and corresponds to the surface tension effects of the compact globule. On fractal lattices, on the contrary, the existence of the stretched exponential factor in the scaling form of HWs is not so straightforward, and such a correspondence cannot be drawn equivalently. In this paper, we reinvestigate the appearance of the stretched exponential factor in the scaling form of HWs on fractal lattices and consider the effects of some kind of 'boundary' condition on it. In particular, in the case of 4-simplex lattice, we explicitly show that the introduction of only two extra links between the corner vertices of the largest generator, leads to complete disappearance of the stretched exponential factor. We also discuss impact of the boundaries on the scaling form of HWs on other fractal lattices.

1. Introduction

Hamiltonian walks (HWs) are classical graph theoretical problem [1]. Being self-avoiding and completely lattice filling, HWs are used to model compact polymer conformations in various situations: polymer collapse [2], polymer melting [3] and protein folding [4,5]. One of the static properties of the HWs problem is the asymptotic form for the number of walks. On two and three dimensional ordinary lattices with open (free) boundary conditions, it is assumed that the number $Z_N$ of $N$-step walks increases with the number of lattice sites $N$, as

$$Z_N \sim \omega^N \mu^N \Gamma^{-1}, \quad N \gg 1.$$  \hspace{1cm} (1)

The exponent $\sigma = \frac{d-1}{d} < 1$ is determined by the lattice dimension $d$ only. Connectivity constant $\omega > 1$ in leading exponential factor, as well as constant $\mu < 1$ in the stretched exponential correction, are both non-universal quantities, i.e. they are lattice dependent. Stretched exponential factor is caused by the boundary sites (surface sites in 3d or perimeter sites in 2d), and is also termed as surface correction. On lattices with periodic boundary conditions, expression similar to (1), with the exception of the stretched exponential, should hold. Formally,
this case is recovered from (1) by setting $\sigma = 0$ or $\mu = 1$. Boundary conditions do not affect the bulk connectivity constant $\omega$, but they do affect the exponent $\gamma$.

The problem of HWs was first studied on the Manhattan oriented square lattice [6,7,8,9], whose directedness enabled an exact approach. Comprehensive treatment conducted by Duplantier and David [9], completely confirmed scaling form (1) for both, closed (circuits) and open walks.

Physically, surface correction in the scaling form (1) represents surface tension effects of the collapsed polymer. Namely, HW model corresponds to a zero temperature limit of the Interacting Self-Avoiding Walk (ISAW) model [2], which represents linear polymer with self-attraction between monomers. Partition function of ISAW model at low temperatures should have the same form as (1), with temperature dependent $\omega$ and $\mu$, as concluded in [10]. The physical reasoning for this conclusion was that collapsed polymer in the form of compact globule has a sharp boundary with the surrounding solvent. Bulk monomers inside the globule interact with other monomers only, while the surface monomers interact with the solvent molecules too. This inconvenient interaction increases free energy of the globule, so that its expected form is: $F = -aN + bN_S$, where $a, b > 0$ are some constants. The first term is contribution from bulk monomers, while the second term accounts for surface correction, with $N_S \propto N^{d-1}$ being the number of surface monomers. As $Z = e^{-F/kT}$, it then follows that partition function should have surface effects, as given in (1). This conclusion was also supported by Monte Carlo simulations in [11].

The problem of HWs has also been studied on fractal lattices [12,13,14,15], where it has been shown that the scaling form, such us (1), does not hold in general. Depending on the fractal lattice, one or both of the corrections can be absent. Moreover, exponent $\sigma$ is not determined by the fractal dimension only [15]. Origin of the stretched exponential factor has been discussed in [15], suggesting that it might have been caused by the lattice sites that have smaller coordination number, but that it is not determined by these sites. Therefore, there is a salient distinction from the case of ordinary lattices (translationally invariant up to a boundaries), where the stretched exponential is caused and determined by the boundary sites. Here, we reexamine the appearance of the stretched exponential in the scaling form of HWs on fractal lattices in particular example of closed HWs on 4-simplex lattice. In section 2, we outline the method for obtaining the asymptotic form. In section 3 we discuss stretched exponential and its possible cause. In the same section, we demonstrate that addition of two extra bonds (as a kind of boundary condition) removes stretched exponential from the scaling form, supporting our previous conjecture that lack of these bonds might have been the reason for its appearance.

![Diagram of 4-simplex lattice](image)

**Figure 1.** The first three steps of construction of 4-simplex lattice. The whole lattice is obtained after infinitely many steps.
2. Scaling form of closed HWs on 4-simplex lattice

4-simplex fractal lattice is constructed iteratively, in infinitely many steps, with the first three shown in figure 1. Structure obtained in the $r$-th step is called $r$-th order generator $G^{(r)}$, which consists of generators of order $r - 1$, and so on. Closed HWs on 4-simplex lattice have been studied in [12], and following these lines, here we outline obtaining of the asymptotic form for the number of walks. Generator of arbitrary order $r + 1$ with schematic representation of all possible closed HWs, is given in figure 2. Closed HWs on $G^{(r+1)}$ consist of walks denoted as $B$, which are open HWs with starting and ending point in the corner vertices of $G^{(r)}$. If the number of all walks $B$ on $G^{(r)}$ is $B_r$, then the number of all closed HWs on $G^{(r+1)}$ can be written as

$$Z^{(c)}_{r+1} = 3(B_r)^4.$$  \hspace{1cm} (2)

The numbers $B_r$ can be expressed recursively, but for the recursion relation to set, one should notice (middle part in figure 2) that walk $B$ on $G^{(r)}$ can visit all lattice sites of $G^{(r-1)}$ by traversing it either once ($B$-type) or twice ($E$-type), so that there are two recurrence equations

$$B_{r+1} = 2B_r^4 + 4B_r^3E_r + 6B_r^2E_r^2,$$
$$E_{r+1} = B_r^4 + 4B_r^3E_r + 22E_r^4.$$  \hspace{1cm} (3)

Initial values $B_1 = 2$ and $E_1 = 1$ are given on the first order generator. Analyzing equations (3) numerically, the following asymptotic behavior has been established: $B_r \ll E_r$,

$$B_r \sim \omega^{N_r} \lambda^{N_r^{1/2}},$$  \hspace{1cm} (4)

and

$$E_r \sim \omega^{N_r},$$  \hspace{1cm} (5)

where $N_r = 4^r$ is the number of sites comprised in $G^{(r)}$. Finally, it was found that the number of closed HWs on $G^{(r)}$ asymptotically grows as

$$Z_{N_r} \sim \omega^{N_r} \mu^{N_r^{1/2}}, N_r \gg 1,$$  \hspace{1cm} (6)

with $\omega = 1.39971$ and $\mu = \lambda^2 = 0.69993$. Thus, correction to the leading order exponential is stretched exponential with $\sigma = \frac{1}{2}$.
3. Effect of corner sites and boundary condition

Before we start to discuss stretched exponential in equation (6), we should first point out some characteristics of the lattice. As one can see in Figure 1, all lattice sites have coordination number four, except for the corner vertices of the largest generator, whose coordination number is three. So, only four lattice sites have smaller coordination number, still, stretched exponential exists. If these four sites give rise to stretched exponential, it is clear that they do not determine it, since this fixed number of sites can be expressed as proportional to $N^0$ (meaning that $\sigma = 0$), while in (6) stands $N^{1/2}$, which is the number of sites along the side or perimeter of the square. But, it has been suggested in reference [15] that the lattice sites with smaller coordination number might cause other lattice sites to appear for HWs as if they also have smaller coordination number.

Now, we will illustrate this idea in the case of 4-simplex lattice, and show that there are actually $\propto N^{1/2}$ sites with effectively smaller coordination number for HWs. In the case of 4-simplex lattice, HWs can traverse some unit square either once or twice in order to visit each of its four sites. If traversed once, we say that this is a unit square with step $B$, and if traversed twice, it is a unit square with step $E$. Since corner vertices of the largest generator have coordination number three, only step $B$ can be realized on each of four unit squares settled in the corners of the largest generator. So, on 4-simplex lattice, it is possible to have closed HWs that consist of all steps $B$, but it is not possible to have HWs with all steps $E$. If we want to build closed HW with maximal number of steps $E$ (maximally entangled closed HW (MEC) [15]), steps $B$ should be placed on at least two sides or two diagonals that connect pairs of corner vertices of the largest generator. These chains of steps $B$ are induced by the $B$ steps on unit squares in the corners of the largest generator, i.e. they are induced by the smaller coordination number of corner vertices. On generator of order $r$, each MEC consists of $2^r$ steps $B$ (there are $2^r$ unit squares with step $B$), and $4^r-1-2^r$ steps $E$. Each of the four sites on unit square with step $E$ is connected through HW with the site on the neighboring unit square, but only two sites on squares with step $B$ have such a connection. Therefore, among all $N_r = 4^r$ sites of the generator of order $r$, there are $2 \cdot 2^r = 2 \cdot N_r^{1/2}$ sites that could be connected through HWs only with the sites on the same unit square, while the rest of the sites can be connected either with the sites on the same or with the sites on the neighboring unit square. In that sense, there are $2 \cdot N_r^{1/2}$ sites with weaker connection through HWs, i.e. with effectively smaller coordination number for HWs (maximally isolated sites [15]). To conclude this part of discussion, in figure 3 we depict a closed maximally entangled HW on $G^{(3)}$. One can notice two sides of the $G^{(3)}$ with steps $B$, and maximally isolated sites shown as grey circles.
Figure 4. Addition of two bonds as a kind of boundary condition (left panel (a)) which enables closed HW that consists of all $E$ steps (right panel (b)).

In order to confirm our conjecture that corner vertices of the largest generator induce maximally isolated sites, we put a boundary condition in such a way that we add two bonds that connect two pairs of corner vertices, as shown in figure 4(a). With these extra bonds, corner vertices have coordination number four, as all other lattice sites. Now, there could be step $E$ on the unit squares in the corners of the largest generator, as well as on all other unit squares. Hence, it is possible to have closed HWs with all steps $E$ (one such walk is schematically shown in figure 4(b)), and all lattice sites can be simultaneously connected through HWs with the sites on neighboring squares. Boundary condition change equation (2), but it does not affect recurrence equations (3), nor asymptotic of walks $B$ and $E$, given with (4) and (5). Expression for the overall number of closed HWs, instead of (2), now has the leading term that is proportional to $(E_r)^4$. It then follows that the asymptotic behavior of the number of closed walks is the same as for the number of walks $E$, which is given by (5). Therefore, asymptotic form for the numbers of closed HWs has only exponential factor, while surface correction is suppressed by the boundary condition. This would be a confirmation of our conjecture that only four sites with smaller coordination number cause stretched exponential on 4-simplex lattice. Very similar reasoning and conclusion can be applied to other $n$-simplex lattices with even $n$, where stretched exponential appeared [14], as well as on the whole family of modified rectangular lattices [16]. But, we make no attempt here to generalize our conclusion straightforwardly to all fractal lattices. Fractal lattices are highly nonhomogeneous, and some lattices can have ‘interior’ sites whose coordination number differs. In this case no ‘boundary’ condition can be involved, and it is not clear how this discrepancy can be removed.

Finally, we would like to mention another difference in behavior of models on ordinary and fractal lattices. Namely, another studied model, also lattice filling, is the closed packed dimer model. Scaling form for the number of dimers on rectangular (or square) lattice consists of leading exponential factor and stretched exponential as perimeter correction [17,18]. But, there is no stretched exponential in the scaling form for the number of dimers on 4-simplex lattice [19]. Thus, only four lattice sites with smaller coordination number have no effect on the scaling form of diatomic molecules on 4-simplex lattice, but they do affect scaling form of long molecules modeled by HWs. This observation is in agreement with our conclusion drawn here that corner sites of 4-simplex lattice induce sites with effectively smaller coordination number with respect to HWs.

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